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(FILE 'HOME' ENTERED AT 08:30:43 ON 01 NOV 2004)

' ENTERED AT 08:30:55 ON 01 NOV 2004

FILE 'REGISTRY' ENTERED AT 08:31:20 ON 01 NOV 2004

FILE 'HCAPLUS' ENTERED AT 08:31:23 ON 01 NOV 2004

L2 TRA L1 1- RN : 11 TERMS

' ENTERED AT 08:31:24 ON 01 NOV 2004

' ENTERED AT 08:31:37 ON 01 NOV 2004

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' ENTERED AT 08:32:06 ON 01 NOV 2004

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FILE COVERS 1907 - 1 Nov 2004 VOL 141 ISS 19

FILE LAST UPDATED: 31 Oct 2004 (20041031/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

L1 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 2003:376823 HCAPLUS  
 DN 138:365147  
 ED Entered STN: 16 May 2003  
 TI Compositions, methods and kits pertaining to luminescent compounds  
 IN Wood, Keith; Hawkins, Erika; Scurria, Mike; Klaubert, Dieter  
 PA Promega Corporation, USA  
 SO PCT Int. Appl., 60 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 IC ICM C07D211-70  
 ICS C07D241-02; C07D413-00; C12N009-02; C12Q001-34; C12Q001-66;  
 G01N033-53  
 CC 9-14 (Biochemical Methods)  
 Section cross-reference(s): 80

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003040100	A1	20030515	WO 2002-US34972	20021101
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2003153090	A1	20030814	US 2001-53482	20011102 <--

Searched by Noble Jarrell

EP 1451155 A1 20040901 EP 2002-802815 20021101  
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK  
PRAI US 2001-53482 A 20011102  
WO 2002-US34972 W 20021101  
CLASS  
PATENT NO. CLASS PATENT FAMILY CLASSIFICATION CODES  
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WO 2003040100 ICM C07D211-70  
ICS C07D241-02; C07D413-00; C12N009-02; C12Q001-34;  
C12Q001-66; G01N033-53  
OS MARPAT 138:365147  
AB A method of measuring the enzymic activity of a luciferase includes  
contacting a luminogenic protein, such as a luciferase, with a protected  
luminophore to form a composition; and detecting light produced from the composition  
The protected luminophore provides increased stability and improved  
signal-to-background ratios relative to the corresponding unmodified  
coelenterazine.  
ST compn kit pertaining luminescent compd protein  
IT Cell  
Luminescent substances  
(comps., methods and kits pertaining to luminescent compds.)  
IT Proteins  
RL: ARU (Analytical role, unclassified); ANST (Analytical study)  
(luminogenic; comps., methods and kits pertaining to luminescent  
compds.)  
IT 61869-41-8, Renilla luciferase  
RL: ARU (Analytical role, unclassified); ANST (Analytical study)  
(comps., methods and kits pertaining to luminescent compds.)  
IT 50909-86-9P 55779-48-1P 65417-16-5P 70217-82-2P 524066-91-9P  
524066-92-0P 524066-93-1P 524066-94-2P 524066-95-3P 524066-96-4P  
RL: ARU (Analytical role, unclassified); SPN (Synthetic preparation); ANST  
(Analytical study); PREP (Preparation)  
(comps., methods and kits pertaining to luminescent compds.)  
RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD  
RE  
(1) Bryan; US 6416960 B1 2002 HCAPLUS  
(2) Garini; US 6165734 A 2000 HCAPLUS  
(3) Hideshi, N; Journal American Chem Society 2001, V123, P1523  
(4) Inouye, S; Biochemical and Biophysical Research Communications 1997, V233,  
P349 HCAPLUS  
(5) Jones, K; Trends in Biotechnology 1999, V17, P477 HCAPLUS  
(6) Roelant; US 6171809 B1 2001 HCAPLUS  
(7) Shimomura, O; Biochemistry Journal 1989, V261, P913 HCAPLUS  
(8) Shimomura, O; Biochemistry Journal 1995, V306, P537 HCAPLUS

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Property values tagged with IC are from the ZIC/VINITI data file  
provided by InfoChem.

STRUCTURE FILE UPDATES: 29 OCT 2004 HIGHEST RN 772333-32-1  
DICTIONARY FILE UPDATES: 29 OCT 2004 HIGHEST RN 772333-32-1

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

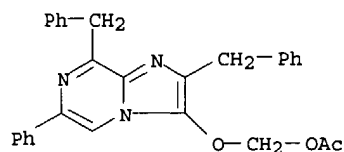
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more  
information enter HELP PROP at an arrow prompt in the file or refer  
to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

L3 ANSWER 1 OF 11 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 524066-96-4 REGISTRY  
CN Methanol, [[6-phenyl-2,8-bis(phenylmethyl)imidazo[1,2-a]pyrazin-3-yl]oxy]-

Searched by Noble Jarrell

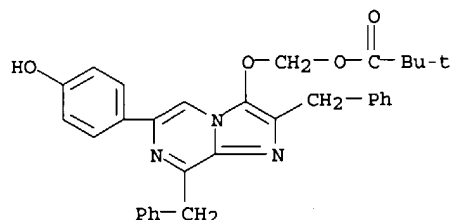
, acetate (ester) (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C29 H25 N3 O3  
 SR CA  
 LC STN Files: CA, CAPLUS, USPATFULL  
 DT.CA Caplus document type: Patent  
 RL.P Roles from patents: ANST (Analytical study); PREP (Preparation)



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 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

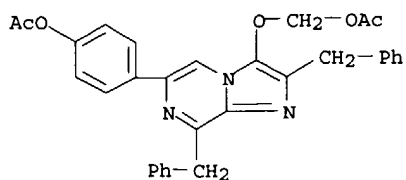
L3 ANSWER 2 OF 11 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 524066-95-3 REGISTRY  
 CN Propanoic acid, 2,2-dimethyl-, [[6-(4-hydroxyphenyl)-2,8-bis(phenylmethyl)imidazo[1,2-a]pyrazin-3-yl]oxy]methyl ester (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C32 H31 N3 O4  
 SR CA  
 LC STN Files: CA, CAPLUS, USPATFULL  
 DT.CA Caplus document type: Conference; Patent  
 RL.P Roles from patents: ANST (Analytical study); PREP (Preparation)  
 RLD.NP Roles for non-specific derivatives from non-patents: BIOL (Biological study); USES (Uses)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

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 1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

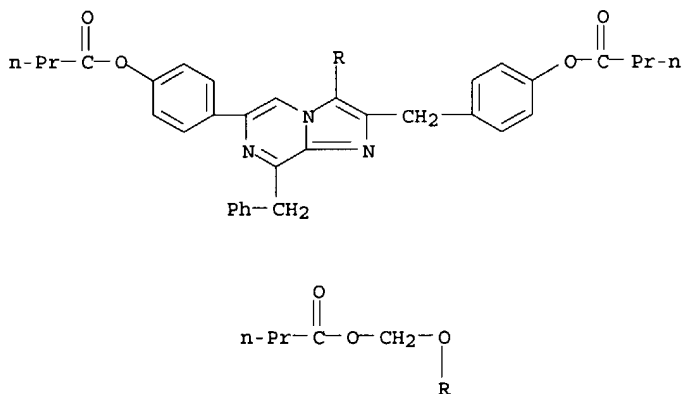
L3 ANSWER 3 OF 11 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 524066-94-2 REGISTRY  
 CN Phenol, 4-[3-[(acetyloxy)methoxy]-2,8-bis(phenylmethyl)imidazo[1,2-a]pyrazin-6-yl]-, acetate (ester) (9CI) (CA INDEX NAME)  
 FS 3D CONCORD  
 MF C31 H27 N3 O5  
 SR CA  
 LC STN Files: CA, CAPLUS, USPATFULL  
 DT.CA Caplus document type: Patent  
 RL.P Roles from patents: ANST (Analytical study); PREP (Preparation)



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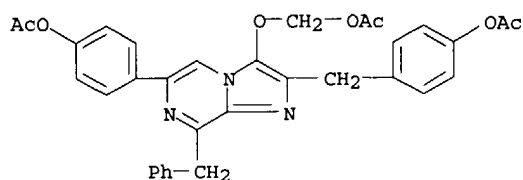
L3 ANSWER 4 OF 11 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 524066-93-1 REGISTRY  
CN Butanoic acid, 4-[3-[(1-oxobutoxy)methoxy]-2-[[4-(1-oxobutoxy)phenyl]methyl]-8-(phenylmethyl)imidazo[1,2-a]pyrazin-6-yl]phenyl ester (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C39 H41 N3 O7  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL  
DT.CA CAplus document type: Patent  
RL.P Roles from patents: ANST (Analytical study); PREP (Preparation)



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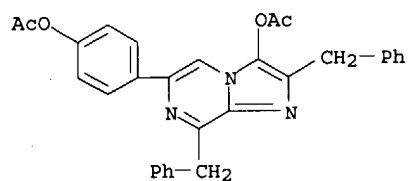
L3 ANSWER 5 OF 11 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 524066-92-0 REGISTRY  
CN Phenol, 4-[3-[(acetyloxy)methoxy]-2-[[4-(acetyloxy)phenyl]methyl]-8-(phenylmethyl)imidazo[1,2-a]pyrazin-6-yl]-, acetate (ester) (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C33 H29 N3 O7  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL  
DT.CA CAplus document type: Patent  
RL.P Roles from patents: ANST (Analytical study); PREP (Preparation)



## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

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1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

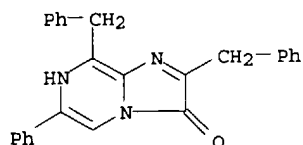
L3 ANSWER 6 OF 11 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 524066-91-9 REGISTRY  
CN Imidazo[1,2-a]pyrazin-3-ol, 6-[4-(acetyloxy)phenyl]-2,8-bis(phenylmethyl)-  
, acetate (ester) (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C30 H25 N3 O4  
SR CA  
LC STN Files: CA, CAPLUS, USPATFULL  
DT.CA Caplus document type: Patent  
RL.P Roles from patents: ANST (Analytical study); PREP (Preparation)



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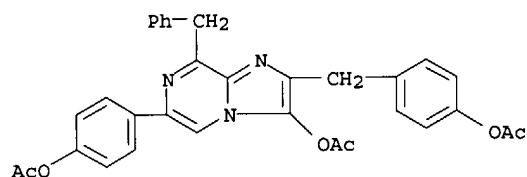
L3 ANSWER 7 OF 11 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 70217-82-2 REGISTRY  
CN Imidazo[1,2-a]pyrazin-3(7H)-one, 6-phenyl-2,8-bis(phenylmethyl)- (9CI)  
(CA INDEX NAME)  
OTHER NAMES:  
CN Bisdeoxycoelenterazine  
CN Coelenterazine 400a  
CN Coelenterazine HH  
CN Dideoxycoelenterazine  
FS 3D CONCORD  
MF C26 H21 N3 O  
LC STN Files: BEILSTEIN\*, CA, CAPLUS, CHEMCATS, CSChem, TOXCENTER, USPAT2,  
USPATFULL  
(\*File contains numerically searchable property data)  
DT.CA Caplus document type: Journal; Patent  
RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study);  
PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or  
reagent); USES (Uses)  
RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation);  
PROC (Process); PRP (Properties); RACT (Reactant or reagent)



## \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

8 REFERENCES IN FILE CA (1907 TO DATE)  
8 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 8 OF 11 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 65417-16-5 REGISTRY  
CN Imidazo[1,2-a]pyrazin-3-ol, 6-[4-(acetyloxy)phenyl]-2-[[4-(acetyloxy)phenyl]methyl]-8-(phenylmethyl)-, acetate (ester) (9CI) (CA INDEX NAME)  
FS 3D CONCORD  
MF C32 H27 N3 O6  
LC STN Files: BEILSTEIN\*, CA, CAPLUS, USPATFULL  
(\*File contains numerically searchable property data)  
DT.CA Caplus document type: Journal; Patent  
RL.P Roles from patents: ANST (Analytical study); PREP (Preparation)  
RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)



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2 REFERENCES IN FILE CA (1907 TO DATE)  
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

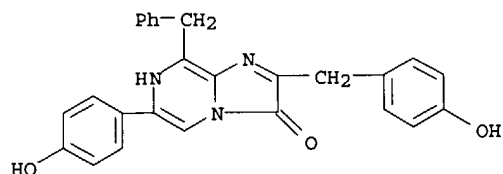
L3 ANSWER 9 OF 11 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 61869-41-8 REGISTRY  
CN Luciferase (Renilla luciferin) (9CI) (CA INDEX NAME)  
OTHER NAMES:  
CN E.C. 1.13.12.5  
CN Luciferase  
CN Renilla luciferase  
CN Renilla luciferin 2-monooxygenase  
MF Unspecified  
CI MAN  
LC STN Files: ADISNEWS, AGRICOLA, BIOSIS, CA, CAPLUS, CEN, CIN, MEDLINE, PIRA, PROMT, TOXCENTER, USPAT2, USPATFULL  
DT.CA Caplus document type: Conference; Dissertation; Journal; Patent; Report  
RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); USES (Uses)  
RLD.P Roles for non-specific derivatives from patents: ANST (Analytical study); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)  
RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation); PROC (Process); PRP (Properties); USES (Uses)  
RLD.NP Roles for non-specific derivatives from non-patents: ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); PRP (Properties); USES (Uses)

## \*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

205 REFERENCES IN FILE CA (1907 TO DATE)  
19 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
208 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 10 OF 11 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 55779-48-1 REGISTRY  
CN Imidazo[1,2-a]pyrazin-3(7H)-one, 6-(4-hydroxyphenyl)-2-[[4-(hydroxyphenyl)methyl]-8-(phenylmethyl)- (9CI) (CA INDEX NAME)  
OTHER NAMES:  
CN Coelenterazin  
CN Coelenterazine  
CN Luciferin

CN Luciferin (Oplophorus)  
 CN NanoFuel  
 CN Preluciferin  
 CN Preluciferin (Watasenia)  
 FS 3D CONCORD  
 DR 57683-96-2  
 MF C26 H21 N3 O3  
 LC STN Files: ADISNEWS, AGRICOLA, BEILSTEIN\*, BIOBUSINESS, BIOSIS, CA, CANCERLIT, CAPLUS, CASREACT, CEN, CHEMCATS, CIN, CSCHM, MEDLINE, PIRA, PROMT, TOXCENTER, USPAT2, USPATFULL  
 (\*File contains numerically searchable property data)  
 DT.CA CAPLUS document type: Conference; Journal; Patent  
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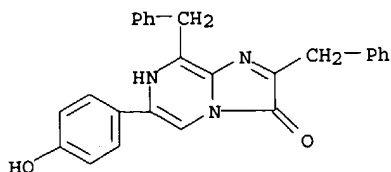
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L3 ANSWER 11 OF 11 REGISTRY COPYRIGHT 2004 ACS on STN  
 RN 50909-86-9 REGISTRY  
 CN Imidazo[1,2-a]pyrazin-3(7H)-one, 6-(4-hydroxyphenyl)-2,8-bis(phenylmethyl)- (9CI) (CA INDEX NAME)

**OTHER NAMES:**

CN 2-Deoxycoelenterazine  
 CN Coelenterazine h  
 CN Luciferin  
 CN Luciferin (Renilla)  
 FS 3D CONCORD  
 DR 50815-16-2  
 MF C26 H21 N3 O2  
 LC STN Files: ADISNEWS, AGRICOLA, BEILSTEIN\*, BIOBUSINESS, BIOSIS, CA, CAPLUS, CEN, CHEMCATS, CIN, CSCHM, MEDLINE, PIRA, PROMT, TOXCENTER, USPATFULL  
 (\*File contains numerically searchable property data)

DT.CA CAPLUS document type: Conference; Journal; Patent  
 RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); PRP (Properties); USES (Uses)  
 RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)  
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 40 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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 COPYRIGHT (C) 2004 THE THOMSON CORPORATION

FILE LAST UPDATED: 27 OCT 2004 <20041027/UP>  
 MOST RECENT DERWENT UPDATE: 200469 <200469/DW>  
 DERWENT WORLD PATENTS INDEX SUBSCRIBER FILE, COVERS 1963 TO DATE

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>>> SMILES and ISOSMILES strings are no longer available as  
 Derwent Chemistry Resource display fields <<<

L4 ANSWER 1 OF 1 WPIX COPYRIGHT 2004 THE THOMSON CORP on STN  
 AN 2003-468516 [44] WPIX  
 DNN N2003-372833 DNC C2003-125061  
 TI Kit useful for measuring the enzymatic activity of a luminogenic protein,  
 comprises a protected luminophore and a luminogenic protein or a  
 deprotecting enzyme.  
 DC B02 B04 D16 S03  
 IN HAWKINS, E; KLAUBERT, D; SCURRIA, M; WOOD, K  
 PA (HAWK-I) HAWKINS E; (KLAU-I) KLAUBERT D; (SCUR-I) SCURRIA M; (WOOD-I) WOOD  
 K; (PROM-N) PROMEGA CORP  
 CYC 102  
 PI WO 2003040100 A1 20030515 (200344)\* EN 30 C07D211-70  
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 MK NL PT RO SE SI SK TR  
 AU 2002363424 A1 20030519 (200464) C07D211-70

Searched by Noble Jarrell



ADT WO 2003040100 A1 WO 2002-US34972 20021101; US 2003153090 A1 US 2001-53482 20011102; EP 1451155 A1 EP 2002-802815 20021101, WO 2002-US34972 20021101; AU 2002363424 A1 AU 2002-363424 20021101

FDT EP 1451155 A1 Based on WO 2003040100; AU 2002363424 A1 Based on WO 2003040100

PRAI US 2001-53482 20011102

IC ICM C07D211-70; G01N021-76

ICS C07D241-02; C07D413-00; C12N009-02; C12Q001-34; C12Q001-66; G01N033-53

AB WO2003040100 A UPAB: 20030710

NOVELTY - A kit comprising a protected luminophore (A) and a luminogenic protein or a deprotecting enzyme, is new.

DETAILED DESCRIPTION - INDEPENDENT CLAIMS are included for:

(1) measurement of an enzymatic activity of a luminogenic protein involves contacting the protein, a deprotecting enzyme and (A) in a solution to form a composition (A1) and detecting the light produced from the composition;

(2) a protected luminophore which is a modified coelenterazine in which the enol group has been converted to an ester or an ether comprising an enzyme-removable group. The removal of the enzyme-removable group provides a parent coelenterazine. The time necessary for the concentration of the modified coelenterazine in a mixture comprising F12 medium and 10% fetal bovine serum at 22 deg. C to be reduced by 50% is greater than the time necessary for the concentration of the parent coelenterazine in a mixture comprising F12 medium and 10% fetal bovine serum at 22 deg. C to be reduced by 50%;

(3) generating luminescence in a living cell comprising the luciferase involves contacting the cell in solution with (A);

(4) measuring the enzymatic activity of a non-luminogenic enzyme involves contacting a liquid mixture comprising the luminogenic protein and (A) to form a composition and detecting the light produced from the composition;

(5) a compound of formula (I) - (III); and

(6) a composition comprising (I) - (III) in solution.

R7 = T or -CH<sub>2</sub>-C<sub>6</sub>H<sub>4</sub>OR<sub>14</sub>;

T = H, (hetero)alkyl or aryl;

R8 = T;

R9 = T or -C<sub>6</sub>H<sub>4</sub>OR<sub>15</sub>;

R10 = H, CH<sub>3</sub> or -CH(CH<sub>3</sub>)<sub>2</sub>;

R11, R14 and R15 = enzyme-removable groups.

Provided that:

(1) R11, R14 and R15 are not all acetyl groups;

(2) the concentration of (I) in a mixture comprising F12 medium and 10% fetal bovine serum at 22 deg. C is reduced by less than 50% after 45 minutes;

(3) in (I), the time necessary for the concentration of the modified coelenterazine in a mixture comprising F12 medium and 10% fetal bovine serum at 22 deg. C to be reduced by 50% is greater than the time necessary for the concentration of the parent coelenterazine in a mixture comprising F12 medium and 10% fetal bovine serum at 22 deg. C to be reduced by 50% and the removal of at least one (preferably at least two, especially all) enzyme-removable groups provides the parent compound.

USE - The kit is used:

(a) for measurement of an enzymatic activity of a luminogenic protein (e.g. Renilla luciferase) and generating luminescence in a living cell comprising luciferase (claimed);

(b) in analytic applications e.g. to detect and quantitate luminogenic analytes which are substrates or proteins and analysis of genetic reporters e.g. multiplexed reporter where at least one reporter utilizes a luminophore;

(c) in in vivo applications within organism, for cell development, to measure a luminogenic analyte or non-luminogenic enzyme in an organ, tissue or cell type;

(d) in in vitro applications to measure substances and processes over time e.g. the expression of the luminogenic protein, the concentration of analyte and the expression of the non-luminogenic enzyme.

ADVANTAGE - The protected luminophore provides increased stability and improved signal-to-background ratio relative to the corresponding unmodified coelenterazine and provides for reduced autoluminescence under normal use conditions and is sensitive to substances other than luminogenic proteins. Therefore the composition is multi-functional and so provides a way to analyze non-luminogenic substances or processes through luminescent methods.

Dwg. 0/3

FS CPI EPI

FA AB; GI; DCN

MC CPI: B04-F01; B04-L01; B04-L03C; B04-N04; B06-D08; B06-D18; B11-C07B4;  
B12-K04E; D05-A01A4; D05-A01B; D05-H09  
EPI: S03-E14H4  
M1 \*01\* DCN: RA00GT-K; RA00GT-Z  
M1 \*02\* DCN: RA0F7A-K; RA0F7A-A; RA0F7A-M  
M1 \*03\* DCN: RA00H3-K; RA00H3-A; RA00H3-M  
M1 \*04\* DCN: RA00GC-K; RA00GC-A; RA00GC-M  
M2 \*05\* DCN: RAAOUX-K; RAAOUX-D; RAAOUX-M  
M2 \*06\* DCN: 0095-66101-K; 0095-66101-D; 0095-66101-M

=> b home  
FILE 'HOME' ENTERED AT 08:32:33 ON 01 NOV 2004

=>

=&gt; b reg

ENTERED AT 09:27:54 ON 01 NOV 2004  
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Property values tagged with IC are from the ZIC/VINITI data file  
 provided by InfoChem.

STRUCTURE FILE UPDATES: 29 OCT 2004 HIGHEST RN 772333-32-1  
 DICTIONARY FILE UPDATES: 29 OCT 2004 HIGHEST RN 772333-32-1

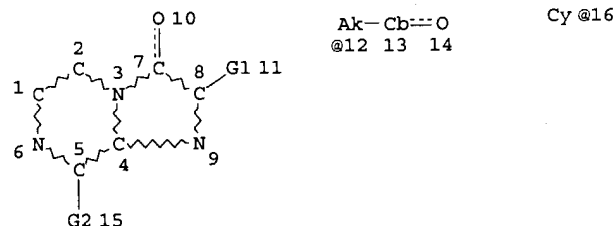
TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when  
 conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more  
 information enter HELP PROP at an arrow prompt in the file or refer  
 to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

L5



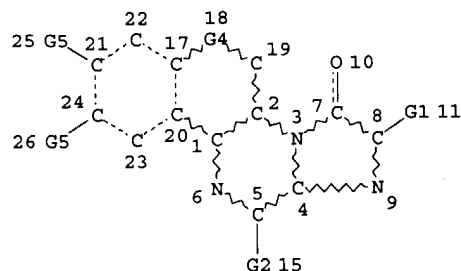
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RSPEC 1  
NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE

100.0% PROCESSED 52 ITERATIONS  
SEARCH TIME: 00.00.01

L11 STR



Ak-Cb---O  
@12 13 14

Cy @16

VAR G1=H/AK/16/12  
VAR G2=H/AK/16  
REP G4=(0-2) C  
VAR G5=H/O/AK/16  
NODE ATTRIBUTES:  
DEFAULT MLEVEL IS ATOM  
GGCAT IS MCY UNS AT 13  
GGCAT IS UNS AT 16  
DEFAULT ECLEVEL IS LIMITED  
ECOUNT IS E6 C AT 13

## GRAPH ATTRIBUTES:

RSPEC 1  
NUMBER OF NODES IS 26

STEREO ATTRIBUTES: NONE

100.0% PROCESSED 2895 ITERATIONS  
SEARCH TIME: 00.00.01

Formula

XIII 6x

XIV

=&gt; d his

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FILE 'HCAPLUS' ENTERED AT 08:30:55 ON 01 NOV 2004

L1 1 US20030153090/PN

FILE 'REGISTRY' ENTERED AT 08:31:20 ON 01 NOV 2004

FILE 'HCAPLUS' ENTERED AT 08:31:23 ON 01 NOV 2004

L2 TRA L1 1- RN : 11 TERMS

FILE 'REGISTRY' ENTERED AT 08:31:24 ON 01 NOV 2004

L3 11 SEA L2

FILE 'WPIX' ENTERED AT 08:31:37 ON 01 NOV 2004

L4 1 US20030153090/PN

FILE 'REGISTRY' ENTERED AT 08:55:54 ON 01 NOV 2004

L5 STR

L6 5 L5

L7 52 L5 FULL

SAVE TEMP GIT482F0/A L7

L8 STR L5

Searched by Noble Jarrell

L9 2 L8 SAM SUB=L7

SAVE TEMP L10 GIT482S0/A

L11 STR L5

L12 0 L11 SAM SUB=L7

L13 0 L11

FILE 'HCAPLUS' ENTERED AT 09:22:14 ON 01 NOV 2004

L15 26 L10

FILE 'HCAOLD' ENTERED AT 09:22:35 ON 01 NOV 2004

L16 0 L10

' ENTERED AT 09:22:40 ON 01 NOV 2004

E WOOD K/AU

L17 225 E3-20

E WOOD KEITH/AU

L18 113 E3-9

E HAWKINS E/AU

L19 78 E3-15

E HAWKINS ERICA/AU

E HAWKINS ERIKA/AU

L20 8 E3-4

E SCURRIA M/AU

L21 4 E4-7

E KLAUBERT D/AU

L22 68 E4-8

L23 249 PROMEGA/CS, PA

L24 3 L15 AND L17-22

L25 3 L15 AND L23

L27 23 L15 AND L26

=> b hcap

ENTERED AT 09:28:14 ON 01 NOV 2004

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FILE COVERS 1907 - 1 Nov 2004 VOL 141 ISS 19  
FILE LAST UPDATED: 31 Oct 2004 (20041031/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

L26 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 2004:270174 HCAPLUS

DN 140:299425

ED Entered STN: 02 Apr 2004

TI Luminescent cytochrome P 450 assay using luciferase, luciferin derivatives and pyrophosphatase, and drug screening applications

Cali, James J.; Klaubert, Dieter; Daily, William; Ho, Samuel Kin Sang; Frackman, Susan; Hawkins, Erika; Wood, Keith V.

Promega Corporation, USA

SO PCT Int. Appl., 130 pp.

CODEN: PIXXD2

DT Patent

LA English

IC ICM G01N

CC 7-1 (Enzymes)

Searched by Noble Jarrell

Section cross-reference(s): 1, 63

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004027378	A2	20040401	WO 2003-US29078	20030916
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004171099	A1	20040902	US 2003-665314	20030919
PRAI US 2002-412254P	P	20020920		
US 2003-483309P	P	20030627		

## CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
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WO 2004027378	ICM	G01N
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OS MARPAT 140:299425

AB The present invention provides methods, compns., substrates, and kits useful for analyzing the metabolic activity in cells, tissue, and animals and for screening test compds. for their effect on cytochrome P 450 activity. In particular, a one-step and two-step methods using luminogenic mols., e.g. luciferin or coelenterazines, that are cytochrome P 450 substrates and that are also bioluminescent enzyme, e.g., luciferase, pro-substrates are provided. Upon addition of the luciferin derivative or other luminogenic mol. into a P 450 reaction, the P 450 enzyme metabolizes the mol. into a bioluminescent enzyme substrate, e.g., luciferin and/or luciferin derivative metabolite, in a P 450 reaction. The resulting metabolite(s) serves as a substrate of the bioluminescent enzyme, e.g., luciferase, in a second light-generating reaction. Luminescent cytochrome P 450 assays with low background signals and high sensitivity are disclosed and isoform selectivity is demonstrated. The present invention also provides an improved method for performing luciferase reactions which employs added pyrophosphatase to remove inorg. pyrophosphate, a luciferase inhibitor which may be present in the reaction mixture as a contaminant or may be generated during the reaction. The present method further provides a method for stabilizing and prolonging the luminescent signal in a luciferase-based assay using luciferase stabilizing agents such as reversible luciferase inhibitors.

ST cytochrome P 450 detn luciferase luciferin coelenterazine bioluminescence; drug screening cytochrome P 450 luminescent assay

IT Animal  
 Animal tissue  
 Bile  
 Cell  
 Feces  
 Liver  
 Microsome  
 (P 450 determination in; luminescent cytochrome P 450 assay using luciferase, luciferin derivs. and pyrophosphatase, and drug screening applications)

IT Transgene  
 RL: BPN (Biosynthetic preparation); BUU (Biological use, unclassified); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (animal, P 450 determination in; luminescent cytochrome P 450 assay using luciferase, luciferin derivs. and pyrophosphatase, and drug screening applications)

IT Enzymes, uses  
 RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)  
 (bioluminescent; luminescent cytochrome P 450 assay using luciferase, luciferin derivs. and pyrophosphatase, and drug screening applications)

IT High throughput screening  
 (drug; luminescent cytochrome P 450 assay using luciferase, luciferin derivs. and pyrophosphatase, and drug screening applications)

IT Drug screening  
 (high throughput; luminescent cytochrome P 450 assay using luciferase, luciferin derivs. and pyrophosphatase, and drug screening applications)

IT Teleostei  
 (in high throughput screening assay; luminescent cytochrome P 450 assay using luciferase, luciferin derivs. and pyrophosphatase, and drug screening applications)

IT Blood analysis  
 Chemiluminescence spectroscopy  
 Chemiluminescent substances  
 Cytolysis  
 High throughput screening  
 Luminescence, bioluminescence  
 Luminescence spectroscopy  
 Luminescent substances  
 Surfactants  
 Test kits  
 Urine analysis  
 (luminescent cytochrome P 450 assay using luciferase, luciferin derivs. and pyrophosphatase, and drug screening applications)

IT Surfactants  
 (nonionic; luminescent cytochrome P 450 assay using luciferase, luciferin derivs. and pyrophosphatase, and drug screening applications)

IT 7048-04-6, Cysteine hydrochloride monohydrate  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (conversion of 2-cyanobenzothiazole derivs. to D-luciferin derivs.; luminescent cytochrome P 450 assay using luciferase, luciferin derivs. and pyrophosphatase, and drug screening applications)

IT 9035-51-2, Cytochrome P 450, biological studies  
 RL: ANT (Analyte); BUU (Biological use, unclassified); ANST (Analytical study); BIOL (Biological study); USES (Uses)  
 (luminescent cytochrome P 450 assay using luciferase, luciferin derivs. and pyrophosphatase, and drug screening applications)

IT 56-65-5, 5'-ATP, uses 2591-17-5D, Luciferin, derivs. 7439-95-4, Magnesium, uses 55779-48-1, Coelenterazine 55779-48-1D, Coelenterazine, derivs. 676460-49-4D, Imidazo[1,2-a]pyrazin-3-ol, derivs.  
 RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)  
 (luminescent cytochrome P 450 assay using luciferase, luciferin derivs. and pyrophosphatase, and drug screening applications)

IT 9014-00-0P, Luciferase 61869-41-8P, Renilla luciferase 61970-00-1P, Firefly luciferase  
 RL: ARG (Analytical reagent use); BPN (Biosynthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (luminescent cytochrome P 450 assay using luciferase, luciferin derivs. and pyrophosphatase, and drug screening applications)

IT 676460-30-3P 676460-31-4P 676460-32-5P 676460-33-6P 676460-34-7P 676460-35-8P 676460-37-0P 676460-39-2P 676460-41-6P 676460-43-8P 676460-47-2P, Coelenterazine HH methyl ether  
 RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)  
 (luminescent cytochrome P 450 assay using luciferase, luciferin derivs. and pyrophosphatase, and drug screening applications)

IT 9024-82-2, Pyrophosphatase  
 RL: ARU (Analytical role, unclassified); ANST (Analytical study)  
 (luminescent cytochrome P 450 assay using luciferase, luciferin derivs. and pyrophosphatase, and drug screening applications)

IT 100-39-0, Benzyl bromide 107-04-0, 1-Bromo-2-chloroethane 402-49-3, 4-(Trifluoromethyl)benzyl bromide 615-20-3, 2-Chlorobenzothiazole 870-63-3, Prenyl bromide 939-69-5, 2-Cyano-6-hydroxybenzothiazole 2591-17-5, D-Luciferin 4916-55-6, 3-(Bromomethyl)pyridine hydrobromide 6138-90-5, Geranyl bromide 31106-82-8, 2-(Bromomethyl)pyridine hydrobromide 73870-24-3, 4-(Bromomethyl)pyridine hydrobromide  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation of 2-cyanobenzothiazole derivs.; luminescent cytochrome P 450 assay using luciferase, luciferin derivs. and pyrophosphatase, and drug screening applications)

IT 103-63-9P, 2-(Bromoethyl)benzene 2602-85-9P, 2-Cyanobenzothiazole 676460-20-1P 676460-21-2P 676460-22-3P 676460-23-4P 676460-24-5P 676460-25-6P 676460-26-7P 676460-27-8P 676460-28-9P 676460-29-0P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of 2-cyanobenzothiazole derivs.; luminescent cytochrome P 450 assay using luciferase, luciferin derivs. and pyrophosphatase, and drug screening applications)

IT 70217-82-2P, Coelenterazine HH  
 RL: ARG (Analytical reagent use); RCT (Reactant); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)  
 (preparation of coelenterazine derivs.; luminescent cytochrome P 450 assay using luciferase, luciferin derivs. and pyrophosphatase, and drug screening applications)

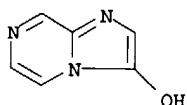
IT 79-37-8, Oxalyl chloride 108-24-7, Acetic anhydride 156-06-9,  
Phenylpyruvic acid 17476-04-9, Lithium tri-tert-butoxyaluminumhydride  
70217-86-6  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(preparation of coelenterazine derivs.; luminescent cytochrome P 450 assay  
using luciferase, luciferin derivs. and pyrophosphatase, and drug  
screening applications)

IT 56485-04-2P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation of coelenterazine derivs.; luminescent cytochrome P 450 assay  
using luciferase, luciferin derivs. and pyrophosphatase, and drug  
screening applications)

IT 92-36-4, 2-(4-Aminophenyl)-6-methylbenzothiazole 2536-91-6,  
2-Amino-6-methylbenzothiazole  
RL: ARU (Analytical role, unclassified); ANST (Analytical study)  
(stabilization of luminescent signal using luciferase inhibitor;  
luminescent cytochrome P 450 assay using luciferase, luciferin derivs.  
and pyrophosphatase, and drug screening applications)

IT 676460-49-4D, Imidazo[1,2-a]pyrazin-3-ol, derivs.  
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)  
(luminescent cytochrome P 450 assay using luciferase, luciferin derivs.  
and pyrophosphatase, and drug screening applications)

RN 676460-49-4 HCAPLUS  
CN Imidazo[1,2-a]pyrazin-3-ol (9CI) (CA INDEX NAME)



L26 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2004 ACS on STN  
AN 2003:376823 HCAPLUS  
DN 138:365147  
ED Entered STN: 16 May 2003  
TI Compositions, methods and kits pertaining to luminescent compounds  
IN Wood, Keith; Hawkins, Erika; Scurria, Mike;  
Klaubert, Dieter  
PA Promega Corporation, USA  
SO PCT Int. Appl., 60 pp.  
CODEN: PIXXD2  
DT Patent  
LA English  
IC ICM C07D211-70  
ICS C07D241-02; C07D413-00; C12N009-02; C12Q001-34; C12Q001-66;  
G01N033-53  
CC 9-14 (Biochemical Methods)  
Section cross-reference(s): 80  
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2003040100	A1	20030515	WO 2002-US34972	20021101
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2003153090	A1	20030814	US 2001-53482	20011102
EP 1451155	A1	20040901	EP 2002-802815	20021101
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
PRAI US 2001-53482	A	20011102		
WO 2002-US34972	W	20021101		

## CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
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WO 2003040100 ICM C07D211-70  
ICS C07D241-02; C07D413-00; C12N009-02; C12Q001-34;  
C12Q001-66; G01N033-53

OS MARPAT 138:365147

AB A method of measuring the enzymic activity of a luciferase includes contacting a luminogenic protein, such as a luciferase, with a protected luminophore to form a composition; and detecting light produced from the composition. The protected luminophore provides increased stability and improved signal-to-background ratios relative to the corresponding unmodified coelenterazine.

ST compn kit pertaining luminescent compd protein

IT Cell  
Luminescent substances  
(comps., methods and kits pertaining to luminescent compds.)

IT Proteins  
RL: ARU (Analytical role, unclassified); ANST (Analytical study)  
(luminogenic; comps., methods and kits pertaining to luminescent compds.)

IT 61869-41-8, Renilla luciferase  
RL: ARU (Analytical role, unclassified); ANST (Analytical study)  
(comps., methods and kits pertaining to luminescent compds.)

IT 50909-86-9P 55779-48-1P 65417-16-5P 70217-82-2P  
524066-91-9P 524066-92-0P 524066-93-1P  
524066-94-2P 524066-95-3P 524066-96-4P  
RL: ARU (Analytical role, unclassified); SPN (Synthetic preparation); ANST  
(Analytical study); PREP (Preparation)  
(comps., methods and kits pertaining to luminescent compds.)

RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD

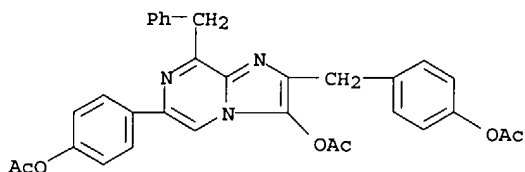
RE

(1) Bryan; US 6416960 B1 2002 HCAPLUS  
(2) Garini; US 6165734 A 2000 HCAPLUS  
(3) Hideshi, N; Journal American Chem Society 2001, V123, P1523  
(4) Inouye, S; Biochemical and Biophysical Research Communications 1997, V233, P349 HCAPLUS  
(5) Jones, K; Trends in Biotechnology 1999, V17, P477 HCAPLUS  
(6) Roelant; US 6171809 B1 2001 HCAPLUS  
(7) Shimomura, O; Biochemistry Journal 1989, V261, P913 HCAPLUS  
(8) Shimomura, O; Biochemistry Journal 1995, V306, P537 HCAPLUS

IT 65417-16-5P  
RL: ARU (Analytical role, unclassified); SPN (Synthetic preparation); ANST  
(Analytical study); PREP (Preparation)  
(comps., methods and kits pertaining to luminescent compds.)

RN 65417-16-5 HCAPLUS

CN Imidazo[1,2-a]pyrazin-3-ol, 6-[4-(acetyloxy)phenyl]-2-[[4-(acetyloxy)phenyl]methyl]-8-(phenylmethyl)-, acetate (ester) (9CI) (CA INDEX NAME)



L26 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 2003:108790 HCAPLUS

DN 139:129758

ED Entered STN: 12 Feb 2003

TI Coelenterazine derivatives for improved solution solubility

AU Hawkins, Erika M.; O'Grady, Michael; Klaubert, Dieter;  
Scurria, Michael; Good, Troy; Stratford, Cathy; Flemming, Rod;  
Simpson, Dan; Wood, Keith V.

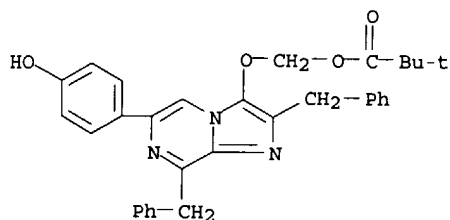
CS Promega Corporation, Madison, WI, 53715, USA

SO Bioluminescence & Chemiluminescence: Progress & Current Applications,  
[Proceedings of the Symposium on Bioluminescence and Chemiluminescence],  
12th, Cambridge, United Kingdom, Apr. 5-9, 2002 (2002), 149-152.  
Editor(s): Stanley, Philip E.; Kricka, Larry J. Publisher: World  
Scientific Publishing Co. Pte. Ltd., Singapore, Singapore.  
CODEN: 69DPGZ; ISBN: 981-238-156-2

DT Conference

LA English

CC 7-3 (Enzymes)  
 Section cross-reference(s): 9  
 AB Intracellular luminescent techniques requiring coelenterazine, such as bioluminescence resonance energy transfer (BRET), calcium detection, and intracellular reporter measurements, must accommodate the poor stability of this substrate in physiol. buffered solns. Coelenterazine degradation leads both to loss of luminescence over time, and increased background luminescence caused by enzyme-independent oxidation (autoluminescence). Both conditions limit luminescence sensitivity by reducing the signal-to-noise ratio. Coelenterazine can be stabilized by derivatizing the enol oxygen with an acyl oxymethyl ether. This prevents spontaneous oxidation in solution while making the substrate available intracellularly upon cleavage of the blocking group by endogenous esterases. We will describe the stability of pivaloyl oxymethyl coelenterazine-h (POM coelenterazine-h), and the effect of POM coelenterazine-h on intracellular luminescence, autoluminescence, and luminescent reaction kinetics. Also, we will present the characteristics of two other coelenterazine derivs.  
 ST coelenterazine deriv improved soln soly reporter  
 IT Luminescence  
 (coelenterazine derivs. for improved solution solubility)  
 IT Animal cell line  
 (mammalian; coelenterazine derivs. for improved solution solubility)  
 IT 50909-86-9, Coelenterazine-h 61869-41-8, Renilla luciferase 524066-95-3D, diacetyl derivative 566945-96-8  
 RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)  
 (coelenterazine derivs. for improved solution solubility)  
 IT 524066-95-3D, diacetyl derivative  
 RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)  
 (coelenterazine derivs. for improved solution solubility)  
 RN 524066-95-3 HCAPLUS  
 CN Propanoic acid, 2,2-dimethyl-, [[6-(4-hydroxyphenyl)-2,8-bis(phenylmethyl)imidazo[1,2-a]pyrazin-3-yl]oxy]methyl ester (9CI) (CA INDEX NAME)



L28 ANSWER 1 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 2001:851130 HCAPLUS  
 DN 135:371764  
 ED Entered STN: 23 Nov 2001  
 TI Preparation of aminopyrazines and imidazolopyrazinones as antioxidants  
 IN Marchand-Brynaert, Jacqueline; Cavalier, Jean-Francois; Rees, Jean-Francois; De Tollenaere, Catherine; Burton, Maggi  
 PA Universite Catholique de Louvain, Belg.  
 SO PCT Int. Appl., 57 pp.  
 CODEN: PIXXD2  
 DT Patent  
 LA English  
 IC ICM C07D241-20  
 ICS A61K031-495; A23L003-3544; C08K005-3462  
 CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))  
 Section cross-reference(s): 1, 17, 38, 62  
 FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2001087853	A1	20011122	WO 2001-EP5588	20010516 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,				

LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU,  
SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,  
YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM  
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,  
DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,  
BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG  
EP 1292580 A1 20030319 EP 2001-943383 20010516 <--  
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR  
US 2004034225 A1 20040219 US 2003-276398 20030728 <--  
PRAI EP 2000-870107 A 20000517 <--  
EP 2000-870293 A 20001212 <--  
WO 2001-EP5588 W 20010516 <--

## CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 2001087853	ICM	C07D241-20
	ICS	A61K031-495; A23L003-3544; C08K005-3462
US 2004034225	ECLA	A23L003/3544; C07D241/20; C07D487/04
OS	CASREACT	135:371764; MARPAT 135:371764
AB	<p>Antioxidants, 5 2-amino-(p-hydroxyphenyl)pyrazines and 3  (p-hydroxyphenyl)-3,7-dihydroimidazo[1,2-a]pyrazin-3-ones were prepared and  claimed useful in diagnostic procedures, as food additives, polymer  additives and as UV screens in cosmetics. E.g., 2-amino-3,5-  dibromopyrazine was treated with p-methoxyphenylboronic acid in the  presence of bis(benzonitrile)palladium dichloride and 1,4-  bis(diphenylphosphino)butane in a solvent mix of EtOH, aqueous sodium  carbonate and toluene to give 66% 2-amino-3,5-bis(p-  methoxyphenyl)pyrazine, which was demethylated with EtSNa in DMF to give  88% 2-amino-3,5-bis(p-hydroxyphenyl)pyrazine (I). In tests on inhibition  of lipid peroxidn. 2-aminopyrazines possessing 2 aryl substituents, one of  them being a p-hydroxyphenyl in o- or p- position with respect to the  amino group, are endowed with antioxidative properties. However, the  p-hydroxyphenyl conferred more activity when located at position 5 than at  position 3. The presence of p-hydroxyphenyl groups at both positions 3  and 5 as in I produced a very active compound. Analogs lacking the free  phenol groups showed reduced activities. Corresponding  imidazolopyrazinones combined the properties of both the  imidazolopyrazinones (delay of the onset of peroxidn.) and the  aminopyrazines (lower rate of oxidation after onset).</p>	
ST	<p>antioxidant aminopyrazine imidazolopyrazinone prepn; food additive  antioxidant aminopyrazine imidazolopyrazinone prepn; polymer additive  antioxidant aminopyrazine imidazolopyrazinone prepn; lipid peroxidn  inhibitor antioxidant aminopyrazine imidazolopyrazinone prepn; UV screen  cosmetic antioxidant aminopyrazine imidazolopyrazinone prepn; pyrazine  amino hydroxyphenyl prepn</p>	
IT	<p>Azines  RL: FFD (Food or feed use); MOA (Modifier or additive use); RCT  (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP  (Preparation); RACT (Reactant or reagent); USES (Uses)  ((p-hydroxyphenyl)pyrazines; preparation of aminopyrazines and  imidazolopyrazinones as antioxidants)</p>	
IT	<p>Polymers, uses  RL: POF (Polymer in formulation); USES (Uses)  (additives; preparation of aminopyrazines and imidazolopyrazinones as  antioxidants)</p>	
IT	<p>Azines  RL: FFD (Food or feed use); MOA (Modifier or additive use); RCT  (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP  (Preparation); RACT (Reactant or reagent); USES (Uses)  (aminopyrazines; preparation of aminopyrazines and imidazolopyrazinones as  antioxidants)</p>	
IT	<p>Lipids, reactions  RL: RCT (Reactant); RACT (Reactant or reagent)  (peroxidn.; preparation of aminopyrazines and imidazolopyrazinones as  antioxidants)</p>	
IT	<p>UV B radiation  (preparation of aminopyrazines and imidazolopyrazinones as antioxidant  protectants against)</p>	
IT	<p>Sunscreens  (preparation of aminopyrazines and imidazolopyrazinones as antioxidant  protectants against UVB radiation)</p>	
IT	<p>Antioxidants  Food additives  Food preservatives  (preparation of aminopyrazines and imidazolopyrazinones as antioxidants)</p>	

IT 350230-59-0P, 2,6-Diamino-3,5-bis(p-hydroxyphenyl)pyrazine 350230-62-5P,  
2-Amino-3,5-bis(p-hydroxyphenyl)pyrazine 374588-71-3P,  
2-Amino-5-(p-hydroxyphenyl)-3-methylpyrazine 374588-73-5P,  
2-Amino-3-(p-hydroxyphenyl)-5-phenylpyrazine  
RL: FFD (Food or feed use); MOA (Modifier or additive use); RCT  
(Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP  
(Preparation); RACT (Reactant or reagent); USES (Uses)  
(preparation of aminopyrazines and imidazolopyrazinones as antioxidants)

IT 350230-61-4P 374588-74-6P 374588-75-7P 374588-76-8P  
374588-77-9P 374588-78-0P  
RL: FFD (Food or feed use); MOA (Modifier or additive use); SPN (Synthetic  
preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of aminopyrazines and imidazolopyrazinones as antioxidants)

IT 19943-97-6P 27955-58-4P  
RL: FFD (Food or feed use); MOA (Modifier or additive use); SPN (Synthetic  
preparation); THU (Therapeutic use); BIOL (Biological study); PREP  
(Preparation); USES (Uses)  
(preparation of aminopyrazines and imidazolopyrazinones as antioxidants)

IT 98-80-6, Phenylboronic acid 100-39-0, Benzyl bromide 5720-07-0,  
p-Methoxyphenylboronic acid 24241-18-7, 2-Amino-3,5-dibromopyrazine  
58885-20-4, 2,6-Diamino-3,5-dibromopyrazine 59489-71-3,  
2-Amino-5-bromopyrazine 67602-05-5, 2-Amino-3-bromo-5-phenylpyrazine  
122775-35-3, 3,4-Dimethoxyphenylboronic acid 350819-24-8,  
2-Amino-3-bromo-5-(4-methoxyphenyl)pyrazine  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(preparation of aminopyrazines and imidazolopyrazinones as antioxidants)

IT 350230-58-9P, 2,6-Diamino-3,5-bis(p-methoxyphenyl)pyrazine 350819-13-5P  
350819-14-6P 374588-70-2P, 2-Amino-5-(p-methoxyphenyl)-3-methylpyrazine  
374588-72-4P, 2-Amino-3-(p-methoxyphenyl)-5-phenylpyrazine 374588-81-5P  
374588-83-7P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation of aminopyrazines and imidazolopyrazinones as antioxidants)

IT 119738-50-0P, 2-Amino-5-(4-methoxyphenyl)pyrazine 174680-63-8P,  
2-Amino-3,5-bis(p-methoxyphenyl)pyrazine  
RL: RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use);  
BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent);  
USES (Uses)  
(preparation of aminopyrazines and imidazolopyrazinones as antioxidants)

IT 57683-97-3P 123488-68-6P 123488-69-7P 144763-52-0P 152719-89-6P  
152719-90-9P 152916-61-5P 350819-19-1P 374588-79-1P  
374588-80-4P 374588-82-6P 374588-84-8P 374588-85-9P  
374588-86-0P 374588-87-1P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of aminopyrazines and imidazolopyrazinones as antioxidants)

IT 13535-13-2P, 2-Amino-5-phenylpyrazine 41270-70-6P, 2-Amino-3,5-  
diphenylpyrazine 73444-23-2P, 2-Methylamino-5-phenylpyrazine  
204770-67-2P, 2-Amino-5-(4-hydroxyphenyl)pyrazine  
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological  
study); PREP (Preparation); USES (Uses)  
(preparation of aminopyrazines and imidazolopyrazinones as antioxidants)

RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD

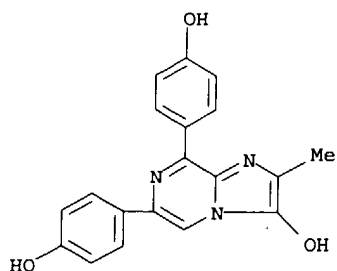
RE

(1) Anon; PATENT ABSTRACTS OF JAPAN 1996, V1996(07)  
(2) Anon; PATENT ABSTRACTS OF JAPAN 1997, V1997(03)  
(3) Anon; PATENT ABSTRACTS OF JAPAN 1998, V1998(08)  
(4) Dubuisson, M; WO 9843641 A 1998 HCAPLUS  
(5) Nippon Oil & JP 08059686 A 1996 HCAPLUS  
(6) Nippon Oil & JP 08294397 A 1996 HCAPLUS  
(7) Nippon Shokuhin Kako Co Ltd; JP 10077286 A 1998 HCAPLUS  
(8) Sato; SYNTHESIS 1994, V9, P931  
(9) Univ Louvain; WO 9628160 A 1996 HCAPLUS  
(10) Watanabe; SYNTHESIS 1980, V1, P39 MEDLINE

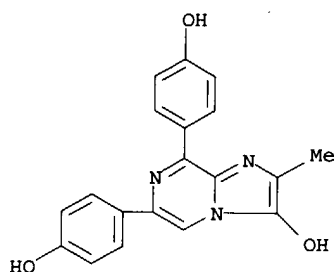
IT 374588-75-7P 374588-76-8P 374588-77-9P  
374588-78-0P  
RL: FFD (Food or feed use); MOA (Modifier or additive use); SPN (Synthetic  
preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of aminopyrazines and imidazolopyrazinones as antioxidants)

RN 374588-75-7 HCAPLUS

CN Imidazo[1,2-a]pyrazin-3-ol, 6,8-bis(4-hydroxyphenyl)-2-methyl- (9CI) (CA  
INDEX NAME)

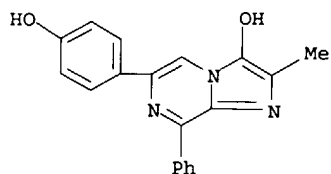


RN 374588-76-8 HCAPLUS  
 CN Imidazo[1,2-a]pyrazin-3-ol, 6,8-bis(4-hydroxyphenyl)-2-methyl-,  
 monohydrochloride (9CI) (CA INDEX NAME)

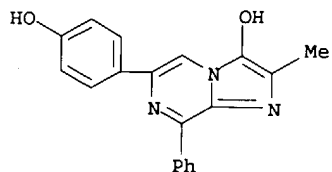


● HCl

RN 374588-77-9 HCAPLUS  
 CN Imidazo[1,2-a]pyrazin-3-ol, 6-(4-hydroxyphenyl)-2-methyl-8-phenyl-,  
 (CA INDEX NAME)



RN 374588-78-0 HCAPLUS  
 CN Imidazo[1,2-a]pyrazin-3-ol, 6-(4-hydroxyphenyl)-2-methyl-8-phenyl-,  
 monohydrochloride (9CI) (CA INDEX NAME)

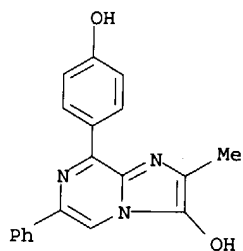


● HCl

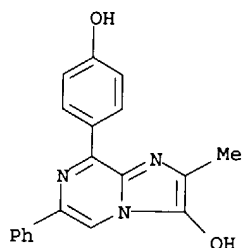
IT 374588-79-1P 374588-80-4P 374588-85-9P  
 374588-86-0P 374588-87-1P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of aminopyrazines and imidazolopyrazinones as antioxidants)

Searched by Noble Jarrell

RN 374588-79-1 HCAPLUS  
 CN Imidazo[1,2-a]pyrazin-3-ol, 8-(4-hydroxyphenyl)-2-methyl-6-phenyl- (9CI)  
 (CA INDEX NAME)

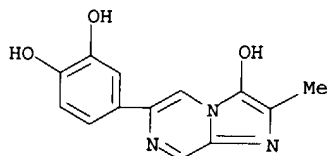


RN 374588-80-4 HCAPLUS  
 CN Imidazo[1,2-a]pyrazin-3-ol, 8-(4-hydroxyphenyl)-2-methyl-6-phenyl-,  
 monohydrochloride (9CI) (CA INDEX NAME)

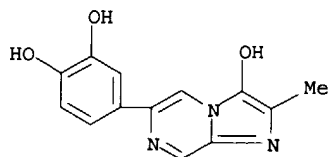


● HCl

RN 374588-85-9 HCAPLUS  
 CN 1,2-Benzenediol, 4-(3-hydroxy-2-methylimidazo[1,2-a]pyrazin-6-yl)- (9CI)  
 (CA INDEX NAME)

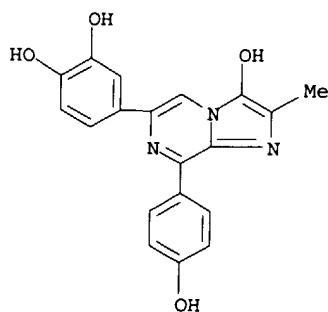


RN 374588-86-0 HCAPLUS  
 CN 1,2-Benzenediol, 4-(3-hydroxy-2-methylimidazo[1,2-a]pyrazin-6-yl)-,  
 monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 374588-87-1 HCAPLUS  
 CN 1,2-Benzenediol, 4-[3-hydroxy-8-(4-hydroxyphenyl)-2-methylimidazo[1,2-a]pyrazin-6-yl]- (9CI) (CA INDEX NAME)



L28 ANSWER 2 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1997:48722 HCAPLUS  
 DN 126:72331  
 ED Entered STN: 23 Jan 1997  
 TI Chemiluminescent substrate for enzyme immunoassay  
 IN Sakaki, Hidejiro; Mitani, Motohiro; Koinuma, Yasuyoshi; Totani, Yoshiaki  
 PA Nippon Oils & Fats Co Ltd, Japan  
 SO Jpn. Kokai Tokkyo Koho, 6 pp.  
 CODEN: JKXXAF  
 DT Patent  
 LA Japanese  
 IC ICM C12Q001-34  
 ICS G01N021-78; G01N033-543  
 CC 9-10 (Biochemical Methods)  
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 08294397	A2	19961112	JP 1995-125617	19950427 <--
PRAI	JP 1995-125617		19950427 <--		

## CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
JP 08294397	ICM	C12Q001-34
	ICS	G01N021-78; G01N033-543

OS MARPAT 126:72331

AB Chemiluminescent substrate for sugar-hydrolyzing enzyme is prepared for EIA. 3-(.beta.-D-galactopyranosyloxy)-6-(4-methoxyphenyl)-2-methylimidazole[1,2-a]pyrazine was prepared from 6-(4-methoxyphenyl)-2-methyl-3-(tetra-O-acetyl-.beta.-D-galactopyranosyloxy)imidazole[1,2-a]pyrazine, and used for chemiluminescent EIA.

ST chemiluminescence EIA substrate carbohydrate hydrolyzing enzyme

IT Immunoglobulins

RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)  
 (G, galactosidase; chemiluminescent substrate for EIA using  
 carbohydrate-hydrolyzing enzyme)

IT Immunoassay

Immunoassay  
 (chemiluminescence enzyme; chemiluminescent substrate for EIA using  
 carbohydrate-hydrolyzing enzyme)

IT 9001-02-9, Carbohydrate-hydrolyzing enzymes 9031-11-2,

.beta.-Galactosidase

RL: ARU (Analytical role, unclassified); ANST (Analytical study)  
 (chemiluminescent substrate for EIA using carbohydrate-hydrolyzing  
 enzyme)

IT 159503-66-9P

RL: ARU (Analytical role, unclassified); SPN (Synthetic preparation); ANST  
 (Analytical study); PREP (Preparation)  
 (chemiluminescent substrate for EIA using carbohydrate-hydrolyzing  
 enzyme)

IT 3068-32-4, 2,3,4,6-Tetra-O-acetyl-.alpha.-D-galactopyranosyl bromide  
 185311-71-1

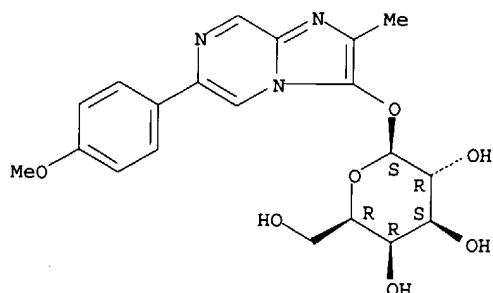
RL: RCT (Reactant); RACT (Reactant or reagent)  
 (chemiluminescent substrate for EIA using carbohydrate-hydrolyzing  
 enzyme)

IT 177205-13-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (chemiluminescent substrate for EIA using carbohydrate-hydrolyzing

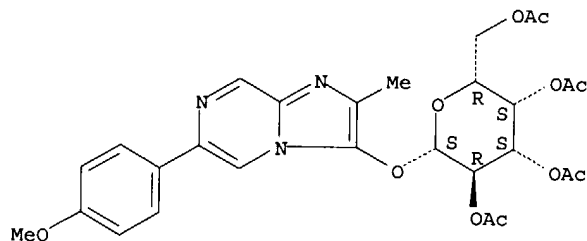
enzyme)  
 IT 159503-66-9P  
 RL: ARU (Analytical role, unclassified); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation)  
 (chemiluminescent substrate for EIA using carbohydrate-hydrolyzing enzyme)  
 RN 159503-66-9 HCAPLUS  
 CN .beta.-D-Galactopyranoside, 6-(4-methoxyphenyl)-2-methylimidazo[1,2-alpyrazin-3-yl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 177205-13-9P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (chemiluminescent substrate for EIA using carbohydrate-hydrolyzing enzyme)  
 RN 177205-13-9 HCAPLUS  
 CN .beta.-D-Galactopyranoside, 6-(4-methoxyphenyl)-2-methylimidazo[1,2-alpyrazin-3-yl, 2,3,4,6-tetraacetate (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L28 ANSWER 3 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1996:335963 HCAPLUS  
 DN 125:11354  
 ED Entered STN: 08 Jun 1996  
 TI Preparation of luciferin derivatives of Umihotaru (Cypridina hilgendorffii)  
 IN Mitani, Motohiro; Sakaki, Hidejiro; Koinuma, Yasuyoshi; Totani, Yoshiaki  
 PA Nippon Oils & Fats Co Ltd, Japan  
 SO Jpn. Kokai Tokkyo Koho, 8 pp.  
 CODEN: JKXXAF  
 DT Patent  
 LA Japanese  
 IC ICM C07H017-02  
 ICS C07D487-04; C12Q001-34; G01N021-78  
 CC 33-3 (Carbohydrates)  
 Section cross-reference(s): 9

FAN.CNT 1

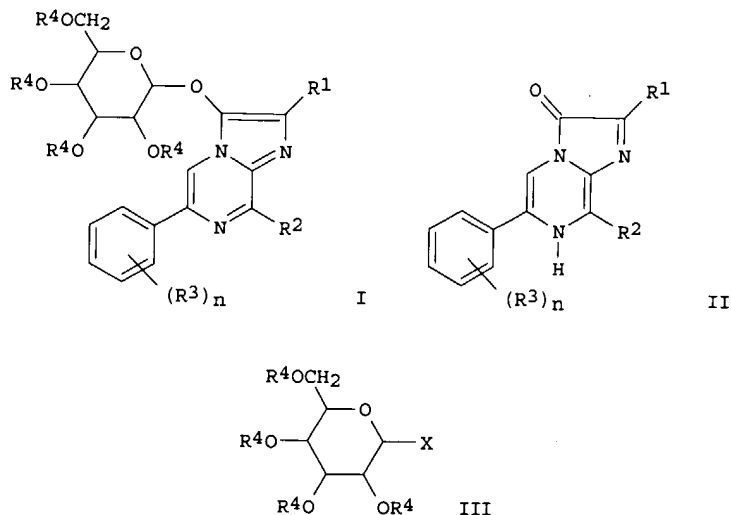
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 08059686	A2	19960305	JP 1994-198770	19940823 <--
JP 1994-198770		19940823 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
JP 08059686	ICM	C07H017-02



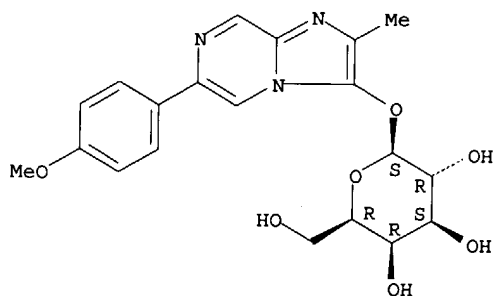
OS ICS C07D487-04; C12Q001-34; G01N021-78  
 GI CASREACT 125:11354; MARPAT 125:11354



- AB The title compds. (I; R1, R2 = H, C1-20 alkyl, C6-20 aryl, C7-19 arylalkyl; R3 = C1-5 alkyl or alkoxy; n = 0-5), which are useful as substrates for luminescent determination of sugar hydrolases such as .alpha.-D-galactosidase, are prepared by reacting imidazopyrazinone derivs. (II; R1 - R3, n = same as above) with sugar derivs. (III; X = halo; R4 = C1-7 acyl) in the presence of silver triflate and Na2HPO4. followed by solvolysis in the presence of an alkali. Thus, 0.1 g 6-(4-methoxyphenyl)-2-methylimidazo[1,2-a]pyrazin-3-one and 1.1 g Na2HPO4 were treated with 5 mL MeCN, 9 mL benzene, and 2.6 g mol. sieve 4A and stirred at room temperature for 1 h, treated with 0.18 g 2,3,4,6-tetra-O-acetyl-.alpha.-D-galactopyranosyl bromide and 0.37 g silver triflate, and stirred at room temperature for 2 h to give 39% 6-(4-methoxyphenyl)-2-methyl-3-(2,3,4,6-tetra-O-acetyl-.alpha.-D-galactopyranosyloxy)imidazo[1,2-a]pyrazine, which (0.5 g) was treated with 3.5 mL MeOH and 1.8 mL concentrated aqueous NH3 and stirred at 40.degree. for 6 h 30 min to give 78% 6-(4-methoxyphenyl)-2-methyl-3-(.alpha.-D-galactopyranosyloxy)imidazo[1,2-a]pyrazine (IV). IV showed luminescence in the presence of .beta.-D-galactosidase with correlation factor r = 0.992.
- ST luciferin deriv Cypridina hilgendorffii prepn; luminescent detn sugar hydrolase; galactosidase luminescent detn substrate luciferin deriv; glucosidase luminescent detn; imidazopyrazinone glycosidation; silver triflate glycosidation catalyst; disodium hydrogen phosphate glycosidation catalyst
- IT Luminescence  
 (preparation of luciferin derivs. of Cypridina hilgendorffii as substrates for luminescent determination of sugar hydrolases)
- IT Glycosidation catalysts  
 (silver triflate and disodium hydrogen phosphate for preparation of luciferin derivs. of Cypridina hilgendorffii by glycosidation of imidazopyrazinones as substrates for luminescent determination of sugar hydrolases)
- IT 9031-11-2  
 RL: ANT (Analyte); ANST (Analytical study)  
 (preparation of luciferin derivs. of Cypridina hilgendorffii as substrates for luminescent determination of sugar hydrolases)
- IT 159503-66-9P 177205-12-8P  
 RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST (Analytical study); PREP (Preparation); USES (Uses)  
 (preparation of luciferin derivs. of Cypridina hilgendorffii as substrates for luminescent determination of sugar hydrolases)
- IT 2923-28-6, Silver triflate 3068-32-4, 2,3,4,6-Tetra-O-acetyl-.alpha.-D-galactopyranosyl bromide 7558-79-4, Disodium hydrogen phosphate  
 RL: CAT (Catalyst use); USES (Uses)  
 (preparation of luciferin derivs. of Cypridina hilgendorffii as substrates

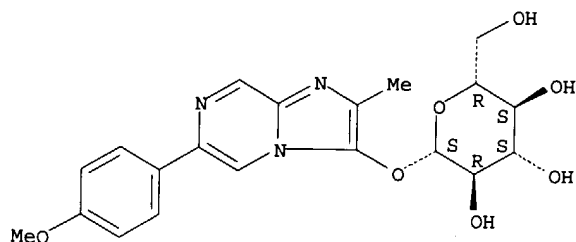
- for luminescent determination of sugar hydrolases)
- IT 572-09-8, 2,3,4,6-Tetra-O-acetyl-.alpha.-D-glucopyranosyl bromide  
118877-07-9  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(preparation of luciferin derivs. of *Cypridina hilgendorffii* as substrates  
for luminescent determination of sugar hydrolases)
- IT 177205-13-9P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation of luciferin derivs. of *Cypridina hilgendorffii* as substrates  
for luminescent determination of sugar hydrolases)
- IT 159503-66-9P 177205-12-8P  
RL: ARG (Analytical reagent use); SPN (Synthetic preparation); ANST  
(Analytical study); PREP (Preparation); USES (Uses)  
(preparation of luciferin derivs. of *Cypridina hilgendorffii* as substrates  
for luminescent determination of sugar hydrolases)
- RN 159503-66-9 HCAPLUS
- CN .beta.-D-Galactopyranoside, 6-(4-methoxyphenyl)-2-methylimidazo[1,2-  
a]pyrazin-3-yl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



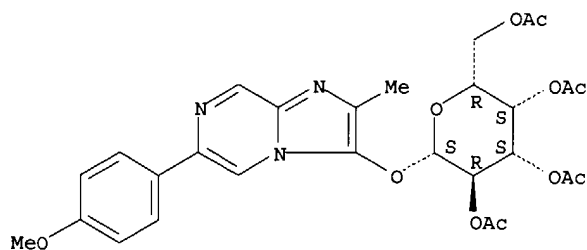
- RN 177205-12-8 HCAPLUS
- CN .beta.-D-Glucopyranoside, 6-(4-methoxyphenyl)-2-methylimidazo[1,2-  
a]pyrazin-3-yl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



- IT 177205-13-9P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation of luciferin derivs. of *Cypridina hilgendorffii* as substrates  
for luminescent determination of sugar hydrolases)
- RN 177205-13-9 HCAPLUS
- CN .beta.-D-Galactopyranoside, 6-(4-methoxyphenyl)-2-methylimidazo[1,2-  
a]pyrazin-3-yl, 2,3,4,6-tetraacetate (9CI) (CA INDEX NAME)

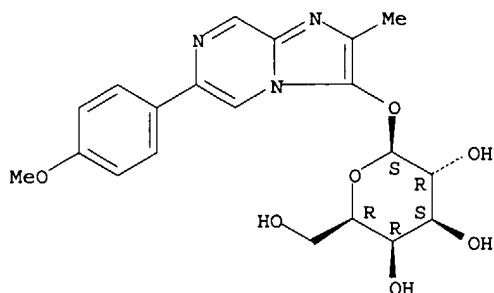
Absolute stereochemistry.



L28 ANSWER 4 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1995:992122 HCAPLUS  
 DN 124:80192  
 ED Entered STN: 20 Dec 1995  
 TI Enhancement effect of 2,6-O-dimethyl-.beta.-cyclodextrin on the  
 chemiluminescent detection of .beta.-D-galactosidase using a Cypridina  
 luciferin analog  
 AU Mitani, Motohiro; Sakaki, Syujiro; Koinuma, Yasumi; Toya, Yoshiaki;  
 Kosugi, Masanori  
 CS Tsukuba Res. Lab., NOF Corp., Tsukuba, 300-26, Japan  
 SO Analytical Sciences (1995), 11(6), 1013-15  
 CODEN: ANSCEN; ISSN: 0910-6340  
 PB Japan Society for Analytical Chemistry  
 DT Journal  
 LA English  
 CC 7-1 (Enzymes)  
 Section cross-reference(s): 9  
 AB .beta.-Cyclodextrins enhanced the chemiluminescent detection of  
 .beta.-galactosidase using the Cypridina luciferin analog  
 3-(.beta.-D-galactopyranosyloxy)-6-(4-methoxyphenyl)-2-methylimidazo[1,2-  
 alpyrazine (.beta.-Gal-MCLA) in the order 2,6-O-dimethyl-.beta.-  
 cyclodextrin > 2,3,6-O-trimethyl-.beta.-cyclodextrin >  
 .beta.-cyclodextrin. Detection of mouse IgG by chemiluminescent enzyme  
 immunoassay (CLEIA) using .beta.-Gal-MCLA and .beta.-galactosidase to  
 amplify the signal was also enhanced by inclusion of 2,6-O-trimethyl-  
 .beta.-cyclodextrin.  
 ST galactosidase beta detn chemiluminescence beta cyclodextrin; IgG detn  
 chemiluminescent enzyme immunoassay cyclodextrin  
 IT Luminescence, chemi-  
 (enhancement effect of 2,6-O-dimethyl-.beta.-cyclodextrin on the  
 chemiluminescent detection of .beta.-D-galactosidase using a Cypridina  
 luciferin analog)  
 IT Immunoglobulins  
 RL: ANT (Analyte); ANST (Analytical study)  
 (G, ant; enhancement effect of 2,6-O-dimethyl-.beta.-cyclodextrin on  
 the chemiluminescent detection of .beta.-D-galactosidase using a  
 Cypridina luciferin analog)  
 IT Immunoassay  
 (chemiluminescence enzyme, enhancement effect of 2,6-O-dimethyl-.beta.-  
 cyclodextrin on the chemiluminescent detection of .beta.-D-  
 galactosidase using a Cypridina luciferin analog)  
 IT 9031-11-2  
 RL: ANT (Analyte); ARG (Analytical reagent use); ANST (Analytical study);  
 USES (Uses)  
 (enhancement effect of 2,6-O-dimethyl-.beta.-cyclodextrin on the  
 chemiluminescent detection of .beta.-D-galactosidase using a Cypridina  
 luciferin analog)  
 IT 7585-39-9, .beta.-Cyclodextrin 51166-71-3, 2,6-O-Dimethyl-.beta.-  
 cyclodextrin 55216-11-0, 2,3,6-O-Trimethyl-.beta.-cyclodextrin  
 159503-66-9  
 RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)  
 (enhancement effect of 2,6-O-dimethyl-.beta.-cyclodextrin on the  
 chemiluminescent detection of .beta.-D-galactosidase using a Cypridina  
 luciferin analog)  
 IT 159503-66-9  
 RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)  
 (enhancement effect of 2,6-O-dimethyl-.beta.-cyclodextrin on the  
 chemiluminescent detection of .beta.-D-galactosidase using a Cypridina  
 luciferin analog)  
 RN 159503-66-9 HCAPLUS  
 CN .beta.-D-Galactopyranoside, 6-(4-methoxyphenyl)-2-methylimidazo[1,2-

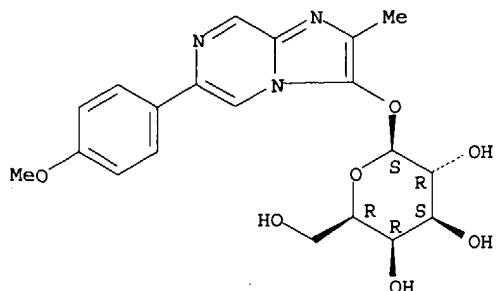
alpyrazin-3-yl (9CI) (CA INDEX NAME)

Absolute stereochemistry.

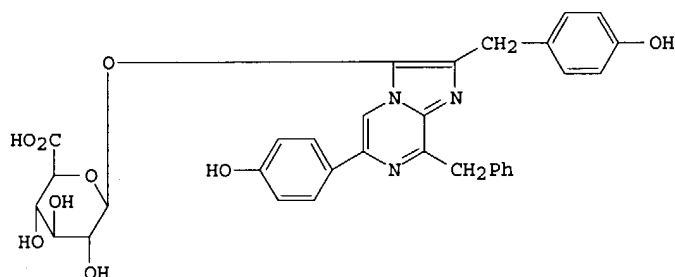


L28 ANSWER 5 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1995:126975 HCAPLUS  
 DN 122:4783  
 ED Entered STN: 08 Nov 1994  
 TI Chemiluminescent assay of .beta.-D-galactosidase using Cypridina luciferin analog: 3-(.beta.-D-galactopyranosyloxy)-6-(4-methoxyphenyl)-2-methylimidazo[1,2-a]pyrazine  
 AU Mitani, Motohiro; Sakaki, Syujiro; Koinuma, Yasumi; Toya, Yoshiaki; Kosugi, Masanori  
 CS Tsukuba Res. Lab., NOF Corp., Ibaraki, 300-26, Japan  
 SO Analytical Sciences (1994), 10(5), 813-14  
 CODEN: ANSCEN; ISSN: 0910-6340  
 DT Journal  
 LA English  
 CC 9-10 (Biochemical Methods)  
 AB We prepared a new Cypridina luciferin analog, 3-(.beta.-D-galactopyranosyloxy)-6-(4-methoxyphenyl)-2-methylimidazo[1,2-a]-pyrazine (.beta.-Gal-MCLA) which can enzymically remove galactose to produce 2-methyl-6-(4-methoxyphenyl)-3,7-dihydroimidazo[1,2-a]pyrazine-3(7H)-one(MCLA), its autoxidn. follows, providing the chemiluminescence. .beta.-Gal-MCLA was thus a useful chemiluminescent substrate for .beta.-D-galactosidase determination  
 ST galactosidase chemiluminescence galactopyranosyloxy methoxyphenyl methylimidazo pyrazine  
 IT 9031-11-2, .beta.-D-Galactosidase  
 RL: ANT (Analyte); ANST (Analytical study)  
 (chemiluminescent assay of .beta.-D-galactosidase using Cypridina luciferin analog: 3-(.beta.-D-galactopyranosyloxy)-6-(4-methoxyphenyl)-2-methylimidazo[1,2-a]pyrazine)  
 IT 159503-66-9  
 RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)  
 (chemiluminescent assay of .beta.-D-galactosidase using Cypridina luciferin analog: 3-(.beta.-D-galactopyranosyloxy)-6-(4-methoxyphenyl)-2-methylimidazo[1,2-a]pyrazine)  
 IT 144465-03-2  
 RL: ARU (Analytical role, unclassified); ANST (Analytical study)  
 (chemiluminescent assay of .beta.-D-galactosidase using Cypridina luciferin analog: 3-(.beta.-D-galactopyranosyloxy)-6-(4-methoxyphenyl)-2-methylimidazo[1,2-a]pyrazine)  
 IT 118877-07-9  
 RL: ARU (Analytical role, unclassified); RCT (Reactant); ANST (Analytical study); RACT (Reactant or reagent)  
 (chemiluminescent assay of .beta.-D-galactosidase using Cypridina luciferin analog: 3-(.beta.-D-galactopyranosyloxy)-6-(4-methoxyphenyl)-2-methylimidazo[1,2-a]pyrazine)  
 IT 159503-66-9  
 RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)  
 (chemiluminescent assay of .beta.-D-galactosidase using Cypridina luciferin analog: 3-(.beta.-D-galactopyranosyloxy)-6-(4-methoxyphenyl)-2-methylimidazo[1,2-a]pyrazine)  
 RN 159503-66-9 HCAPLUS  
 CN .beta.-D-Galactopyranoside, 6-(4-methoxyphenyl)-2-methylimidazo[1,2-a]pyrazin-3-yl (9CI) (CA INDEX NAME)

Absolute stereochemistry.



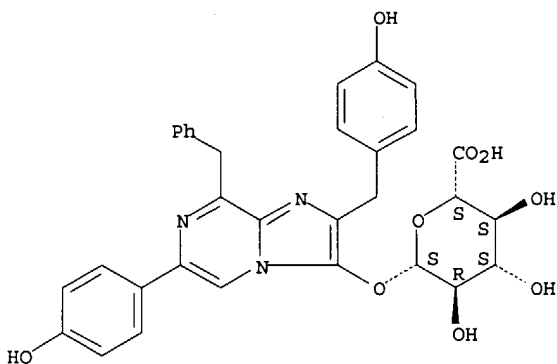
L28 ANSWER 6 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1987:153383 HCAPLUS  
 DN 106:153383  
 ED Entered STN: 15 May 1987  
 TI Chemical studies of myctophina fish bioluminescence  
 AU Inoue, Shoji; Okada, Kunisuke; Tanino, Hideo; Kakoi, Hisae  
 CS Fac. Pharm., Meijo Univ., Nagoya, 468, Japan  
 SO Chemistry Letters (1987), (2), 417-18  
 CODEN: CMLTAG; ISSN: 0366-7022  
 DT Journal  
 LA English  
 CC 12-1 (Nonmammalian Biochemistry)  
 Section cross-reference(s): 26  
 GI



I

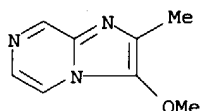
AB A new type of masked watasenia preluciferin was isolated from the liver of a myctophina fish (Diaphus elucens) and its structure was determined as watasenia preluciferinyl .beta.-D-glucopyranosiduronic acid (I).  
 ST Diaphus liver watasenia preluciferinyl glucopyranosidurate; myctophina fish watasenia preluciferinyl glucopyranosidurate  
 IT Diaphus elucens  
 (watasenia preluciferinyl glucopyranosidurate of liver of)  
 IT Liver, composition  
 (watasenia preluciferinyl glucopyranosidurate of, of myctophina fish)  
 IT 107503-11-7  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (deacetylation of)  
 IT 65417-18-7  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (esterification of)  
 IT 107503-09-3  
 RL: BIOL (Biological study)  
 (of liver, of myctophina fish)  
 IT 55779-48-1P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of)  
 IT 107503-11-7  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (deacetylation of)  
 RN 107503-11-7 HCAPLUS  
 CN .beta.-D-Glucopyranosiduronic acid, 6-[4-(acetyloxy)phenyl]-2-[[4-(acetyloxy)phenyl]methyl]-8-(phenylmethyl)imidazo[1,2-a]pyrazin-3-yl (9CI)  
 (CA INDEX NAME)

Absolute stereochemistry.



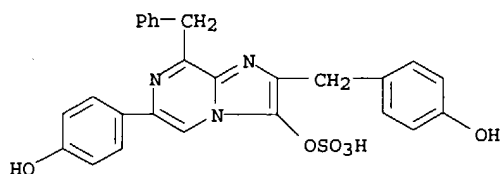
Searched by Noble Jarrell

carbon-13 NMR identification of)  
 IT Spectrochemical analysis  
 (NMR, carbon-13, in identification of Me derivs. of tautomeric hydroxy  
 and mercapto nitrogen heterocyclic compds.)  
 IT Heterocyclic compounds  
 RL: ANST (Analytical study)  
 (nitrogen, identification of Me derivs. of tautomeric hydroxy and  
 mercapto, carbon-13 NMR spectrometric)  
 IT 83-54-5 142-08-5 557-01-7 620-08-6 626-64-2 694-85-9 695-19-2  
 823-09-6 931-63-5 1628-89-3 1722-10-7 2044-27-1 2228-30-0  
 2637-34-5 3739-81-9 4556-23-4 4562-27-0 6104-41-2 6104-45-6  
 6104-46-7 6887-59-8 18438-38-5 22581-72-2 53745-18-9 73547-86-1  
 79690-90-7 79690-93-0 87814-34-4 87814-37-7 **87814-38-8**  
 94317-79-0 94317-80-3  
 RL: ANST (Analytical study)  
 (identification of, carbon-13 NMR spectrometric)  
 IT **87814-38-8**  
 RL: ANST (Analytical study)  
 (identification of, carbon-13 NMR spectrometric)  
 RN 87814-38-8 HCAPLUS  
 CN Imidazo[1,2-a]pyrazine, 3-methoxy-2-methyl- (9CI) (CA INDEX NAME)



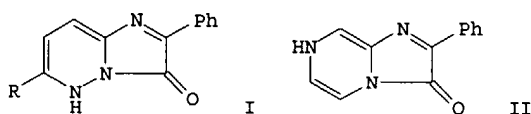
L28 ANSWER 8 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1984:468065 HCAPLUS  
 DN 101:68065  
 ED Entered STN: 01 Sep 1984  
 TI Mechanism of photoinactivation and re-activation in the bioluminescence  
 system of the ctenophore Mnemiopsis  
 AU Anctil, Michel; Shimomura, Osamu  
 CS Mar. Biol. Lab., Woods Hole, MA, 02543, USA  
 SO Biochemical Journal (1984), 221(1), 269-72  
 CODEN: BIJOAK; ISSN: 0306-3275  
 DT Journal  
 LA English  
 CC 6-3 (General Biochemistry)  
 Section cross-reference(s): 12  
 AB The bioluminescence of *M. leidyi* takes place when the photoprotein  
 mnemiopsin in the photocytes reacts with Ca<sup>2+</sup>. The luminescence is  
 inhibited in sunlight and this photoinhibition is reversible by keeping  
 the live specimens in the dark. Exts. of mnemiopsin are similarly  
 photoinhibited, but the photoinhibition cannot be reversed in the dark.  
 Photoinhibited mnemiopsin can be reactivated in the dark by incubation  
 with coelenterazine and O only in solns. having a pH very close to 9.0.  
 The reactivation in vivo probably takes place in the same manner, using  
 the coelenterazine that is supplied from its abundant storage form.  
 Apparently, photoinactivation of mnemiopsin results in the dissociation of  
 coelenterazine and O from the mol. of photoprotein; the dissociated form of  
 the former mol. is an inactive form of coelenterazine, not free  
 coelenterazine.  
 ST bioluminescence Mnemiopsis photoinactivation; mnemiopsin light  
 inactivation coelenterazine oxygen; ctenophore bioluminescence  
 photoinactivation; luminescence bio Mnemiopsis  
 IT Light, biological effects  
 (bioluminescence of ctenophore inactivation by, reactivation by  
 coelenterazine and oxygen in relation to)  
 IT Mnemiopsis leidyi  
 (bioluminescence of, light inactivation of, reactivation by  
 coelenterazine and oxygen in relation to)  
 IT Luminescence, bio-  
 (of ctenophore, light inactivation of, reactivation by coelenterazine  
 and oxygen in relation to)  
 IT Proteins  
 RL: BIOL (Biological study)  
 (mnemiopsins, light inactivation of, reactivation by coelenterazine and  
 oxygen in relation to)  
 IT 7782-44-7, biological studies  
 RL: BIOL (Biological study)

(mnemiopsin activation by coelenterazine and)  
 IT 55779-48-1  
 RL: BIOL (Biological study)  
 (mnemiopsin activation by oxygen and)  
 IT 55779-48-1D, oxidized 65417-14-3  
 RL: BIOL (Biological study)  
 (of ctenophore)  
 IT 65417-14-3  
 RL: BIOL (Biological study)  
 (of ctenophore)  
 RN 65417-14-3 HCAPLUS  
 CN Imidazo[1,2-a]pyrazin-3-ol, 6-(4-hydroxyphenyl)-2-[(4-hydroxyphenyl)methyl]-8-(phenylmethyl)-, 3-(hydrogen sulfate), monosodium salt (9CI) (CA INDEX NAME)



● Na

L28 ANSWER 9 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1983:594926 HCAPLUS  
 DN 99:194926  
 ED Entered STN: 12 May 1984  
 TI Imidazo[1,2-b]pyridazines and an imidazo[1,2-a]pyrazine from pyridazin- and pyrazinamines  
 AU Barlin, Gordon B.; Brown, Desmond J.; Kadunc, Zdenka; Petric, Andrej; Stanovnik, Branka; Tisler, Miha  
 CS John Curtin Sch. Med. Res., Canberra, 2601, Australia  
 SO Australian Journal of Chemistry (1983), 36(6), 1215-20  
 CODEN: AJCHAS; ISSN: 0004-9425  
 DT Journal  
 LA English  
 CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))  
 OS CASREACT 99:194926  
 GI



AB The ambiguous condensations of PhCOCHO with pyridazin-3-amines and pyrazin-2-amine give imidazopyridazinones I (R = H, Cl) and imidazopyrazinone II; resp. The former products exist as such, at least in the solid state, whereas the latter product exists to a large extent as the corresponding dipolar mol. The reactions, degrdms., and NMR spectra of the products are discussed.  
 ST imidazopyrazine; imidazopyridazine; phenylglyoxal cyclization  
 pyridazinamine pyrazinamine  
 IT 6342-56-9  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cyclization of, with chloropyridinamine, imidazopyrazidine derivative)  
 IT 5469-69-2 5469-70-5  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cyclization of, with phenylglyoxal, imidazopyrazinone derivative from)  
 IT 5049-61-6  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cyclization of, with phenylglyoxal, phenylimidazolpyrazinone from)  
 IT 1074-12-0  
 RL: RCT (Reactant); RACT (Reactant or reagent)

Searched by Noble Jarrell



(cyclization of, with pyridazinamines and pyrazinamines, imidazolpyrazinone and imidazopyrazinone derivs. from)

IT 87814-32-2P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and methylation of)

IT 87814-31-1P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and reactions of)

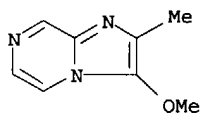
IT 27955-58-4P 87814-33-3P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and ring cleavage of)

IT 87814-34-4P 87814-35-5P 87814-36-6P 87814-37-7P 87814-38-8P  
87814-39-9P 87814-40-2P 87814-41-3P 87814-42-4P 87814-43-5P  
87814-44-6P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

IT 87814-38-8P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 87814-38-8 HCAPLUS

CN Imidazo[1,2-a]pyrazine, 3-methoxy-2-methyl- (9CI) (CA INDEX NAME)



L28 ANSWER 10 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1980:107639 HCAPLUS

DN 92:107639

ED Entered STN: 12 May 1984

TI Comparison of the amounts of key components in the bioluminescence systems of various coelenterates

AU Shimomura, Osamu; Johnson, Frank H.

CS Dep. Biol., Princeton Univ., Princeton, NJ, 08540, USA

SO Comparative Biochemistry and Physiology, Part B: Biochemistry & Molecular Biology (1979), 64B(1), 105-7

CODEN: CBPBB8; ISSN: 0305-0491

DT Journal

LA English

CC 12-1 (Nonmammalian Biochemistry)

AB Luciferase, photoprotein, free and protein-bound coelenterazine (I) and I enol-sulfate were assayed and compared in 5 bioluminescent coelenterates. Hydrozoans Aequorea aequorea and Halistaura cellularia contained photoprotein plus very small amts. of I enol-sulfate and luciferase activity, but no free I. Anthozoans Ptilosarcus gurneyi, Cavernularia obesa, and Renilla muelleri contained luciferase, I, and I enol-sulfate, but very little or no photoprotein. I existed mainly in a stabilized form bound to a Ca-binding protein. The bioluminescent reactions in the coelenterates were compared.

ST bioluminescence coelenterate; luciferase coelenterate bioluminescence; coelenterazine coelenterate bioluminescence; photoprotein coelenterate bioluminescence

IT Aequorea aequorea  
Cavernularia obesa  
Coelenterate  
Halistaura cellularia  
Ptilosarcus gurneyi  
Renilla muelleri  
(bioluminescence system components of)

IT Luminescence, bio-  
(in coelenterates)

IT Proteins  
RL: BIOL (Biological study)  
(photo-, of coelenterates, bioluminescence in relation to)

IT 9014-00-0 55779-47-0 55779-48-1  
RL: BIOL (Biological study)  
(of coelenterates, bioluminescence in relation to)

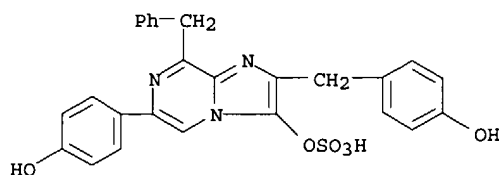
IT 55779-47-0

RL: BIOL (Biological study)

(of coelenterates, bioluminescence in relation to)

RN 55779-47-0 HCAPLUS

CN Imidazo[1,2-a]pyrazin-3-ol, 6-(4-hydroxyphenyl)-2-[(4-hydroxyphenyl)methyl]-8-(phenylmethyl)-, 3-(hydrogen sulfate) (9CI) (CA INDEX NAME)



L28 ANSWER 11 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1979:519858 HCAPLUS

DN 91:119858

ED Entered STN: 12 May 1984

TI A Bioluminescence assay for PAP (3',5'-diphosphoadenosine) and PAPS (3'-phosphoadenylyl sulfate)

AU Anderson, James Michael; Hori, Kazuo; Cormier, Milton J.

CS Boyd Grad. Stud. Res. Cent., Univ. Georgia, Athens, GA, 30602, USA

SO Methods in Enzymology (1978), 57(Biolumin. Chemilumin.), 244-57

CODEN: MENZAU; ISSN: 0076-6879

DT Journal

LA English

CC 9-6 (Biochemical Methods)

AB Procedures in the bioluminescence assay of PAP and PAPS using the luciferin-luciferase reaction in Renilla reniformis are described. The assay is sensitive to 0.1 pmol of PAP. The synthesis of the substrate benzyl luciferin sulfate and isolation of luciferin sulfokinase and luciferase are also described.

ST diphosphoadenosine detn bioluminescence assay; PAPS detn bioluminescence

IT Spinach

(diphosphoadenosine and PAPS determination in leaves of, bioluminescence assay for)

IT Heart, composition

Kidney, composition

Liver, composition

Lung, composition

Photobacterium fischeri

(diphosphoadenosine and PAPS determination in, bioluminescence assay for)

IT Potato

(diphosphoadenosine and PAPS determination in tubers of, bioluminescence assay for)

IT Renilla reniformis

(luciferase and luciferin sulfokinase isolation from, for

diphosphoadenosine and PAPS bioluminescence assay)

IT 71369-26-1

RL: ANST (Analytical study)

(condensation of, with aminobenzylmethoxyphenylpyrazine Me ether)

IT 40040-81-1

RL: ANST (Analytical study)

(condensation of, with benzyl glyoxal di-Et acetal)

IT 482-67-7 1053-73-2

RL: ANT (Analyte); ANST (Analytical study)

(determination of, bioluminescence assay for)

IT 9014-00-0 37278-33-4

RL: PROC (Process)

(isolation of, of Renilla reniformis for diphosphoadenosine and PAPS bioluminescence assay)

IT 50909-83-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(preparation and demethylation of)

IT 71369-28-3P

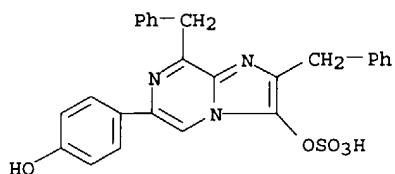
RL: PREP (Preparation)

(preparation of, as substrate for diphosphoadenosine and PAPS bioluminescence assay)

IT 71369-27-2

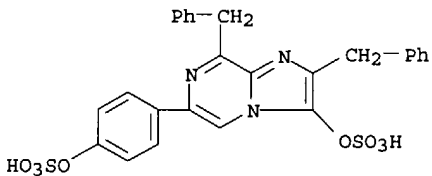
RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with aryl sulfatase)  
 IT 9016-17-5  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with benzyl luciferyl disulfate)  
 IT 50909-86-9  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (sulfonation of)  
 IT 71369-28-3P  
 RL: PREP (Preparation)  
 (preparation of, as substrate for diphosphoadenosine and PAPS  
 bioluminescence assay)  
 RN 71369-28-3 HCAPLUS  
 CN Imidazo[1,2-a]pyrazin-3-ol, 6-(4-hydroxyphenyl)-2,8-bis(phenylmethyl)-,  
 3-(hydrogen sulfate), monopotassium salt (9CI) (CA INDEX NAME)



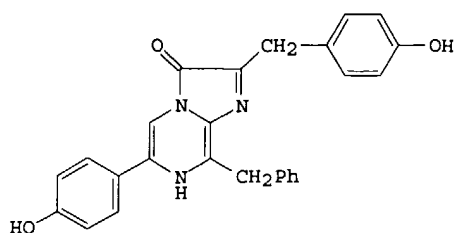
● K

IT 71369-27-2  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (reaction of, with aryl sulfatase)  
 RN 71369-27-2 HCAPLUS  
 CN Imidazo[1,2-a]pyrazin-3-ol, 2,8-bis(phenylmethyl)-6-[4-(sulfooxy)phenyl]-,  
 hydrogen sulfate (ester), dipotassium salt (9CI) (CA INDEX NAME)

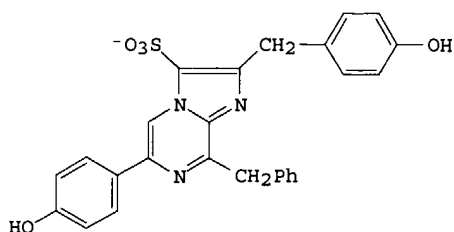


● 2 K

L28 ANSWER 12 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1978:50764 HCAPLUS  
 DN 88:50764  
 ED Entered STN: 12 May 1984  
 TI Complete structure of Renilla luciferin and luciferyl sulfate  
 AU Inoue, Shoji; Kakoi, Hisae; Murata, Mikiko; Goto, Toshio; Shimomura, Osamu  
 CS Fac. Pharm., Meijo Univ., Nagoya, Japan  
 SO Tetrahedron Letters (1977), (31), 2685-8  
 CODEN: TELEAY; ISSN: 0040-4039  
 DT Journal  
 LA English  
 CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))  
 GI



I



II

AB Examination of Renilla exts. showed that Renilla luciferin is coelenterazine (I). The structure of natural luciferyl sulfate was determined as II by comparison of natural and synthetic II. II was synthesized from I by sequential treatment with (AcO)<sub>2</sub>O, MeOH/NH<sub>3</sub>, and pyridine-SO<sub>3</sub> complex and hydrolysis with MeOH/NaOH.

ST Renilla luciferin structure; luciferyl sulfate Renilla prepn

IT 65417-16-5P 65417-17-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and hydrolysis of)

IT 65417-14-3P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(preparation and structure of)

IT 65417-18-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and sulfonation of)

IT 61369-28-6P 65417-15-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

IT 55779-48-1

RL: RCT (Reactant); RACT (Reactant or reagent)

(structure, sulfonylation, and acetylation of)

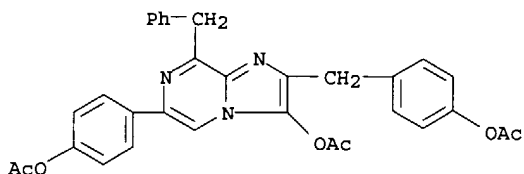
IT 65417-16-5P 65417-17-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and hydrolysis of)

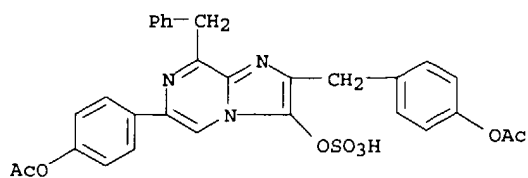
RN 65417-16-5 HCAPLUS

CN Imidazo[1,2-a]pyrazin-3-ol, 6-[4-(acetyloxy)phenyl]-2-[[4-(acetyloxy)phenyl]methyl]-8-(phenylmethyl)-, acetate (ester) (9CI) (CA INDEX NAME)



RN 65417-17-6 HCAPLUS

CN Imidazo[1,2-a]pyrazin-3-ol, 6-[4-(acetyloxy)phenyl]-2-[[4-(acetyloxy)phenyl]methyl]-8-(phenylmethyl)-, hydrogen sulfate (ester), sodium salt (9CI) (CA INDEX NAME)



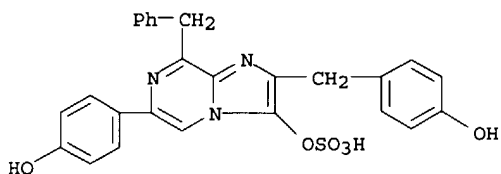
● Na

IT 65417-14-3P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
(preparation and structure of)

RN 65417-14-3 HCAPLUS

CN Imidazo[1,2-a]pyrazin-3-ol, 6-(4-hydroxyphenyl)-2-[(4-hydroxyphenyl)methyl]-8-(phenylmethyl)-, 3-(hydrogen sulfate), monosodium salt (9CI) (CA INDEX NAME)

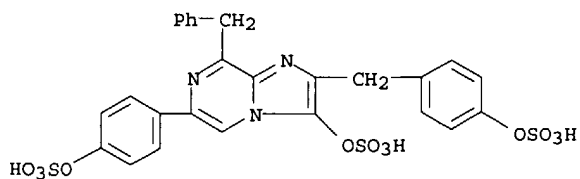


● Na

IT 65417-15-4P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 65417-15-4 HCAPLUS

CN Imidazo[1,2-a]pyrazin-3-ol, 8-(phenylmethyl)-6-[4-(sulfooxy)phenyl]-2-[(4-(sulfooxy)phenyl)methyl]-, hydrogen sulfate (ester), trisodium salt (9CI)  
(CA INDEX NAME)

● 3 Na

L28 ANSWER 13 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 1977:596264 HCAPLUS

DN 87:196264

ED Entered STN: 12 May 1984

TI Substrate and substrate analog binding properties of Renilla luciferase

AU Matthews, John C.; Hori, Kazuo; Cormier, Milton J.

CS Dep. Biochem., Univ. Georgia, Athens, GA, USA

SO Biochemistry (1977), 16(24), 5217-20

CODEN: BICHAW; ISSN: 0006-2960

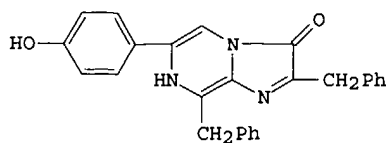
DT Journal

LA English

CC 7-3 (Enzymes)

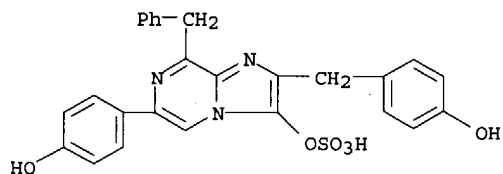
GI

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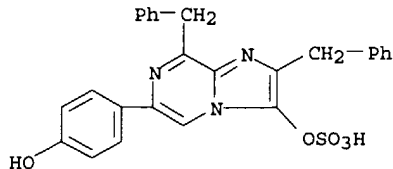


I

- AB The binding characteristics of luciferin, luciferin analogs (e.g. I), and competitive inhibitors of the luciferin-luciferase reaction were studied. Luciferin binding and orientation in the single luciferin binding site of luciferase from *R. reniformis* are highly specific for and dependent upon the 3 group substituents of the luciferin mol., whereas the imidazolone-pyrazine nucleus of luciferin is not directly involved in binding. Anaerobic luciferin binding promotes a rapid concentration-dependent aggregation of luciferase which results in irreversible inactivation of the enzyme. This aggregation phenomenon is not observed upon binding of oxyluciferin, luciferyl sulfate, or luciferin analogs in which the substituent at the 2 position of the imidazolone-pyrazine ring has been substantially altered.
- ST luciferase substrate analog binding; Renilla luciferase substrate binding
- IT Renilla reniformis  
(luciferase of, inhibitor and substrate binding by)
- IT Kinetics, enzymic  
(of inhibition, of luciferase)
- IT 51-67-2 100-46-9, reactions 103-49-1 104-94-9 108-88-3, reactions 108-95-2, reactions 6373-46-2 17297-75-5 19943-97-6 37156-84-6 40040-83-3 50909-85-8 50909-86-9 55779-47-0 55779-48-1 64750-82-9 64750-83-0 64750-84-1
- RL: PROC (Process)  
(luciferase binding of, structural factors in)
- IT 9014-00-0  
RL: BIOL (Biological study)  
(of Renilla, inhibitor and substrate binding by, structural factors in)
- IT 55779-47-0 64750-83-0  
RL: PROC (Process)  
(luciferase binding of, structural factors in)
- RN 55779-47-0 HCAPLUS
- CN Imidazo[1,2-a]pyrazin-3-ol, 6-(4-hydroxyphenyl)-2-[(4-hydroxyphenyl)methyl]-8-(phenylmethyl)-, 3-(hydrogen sulfate) (9CI) (CA INDEX NAME)

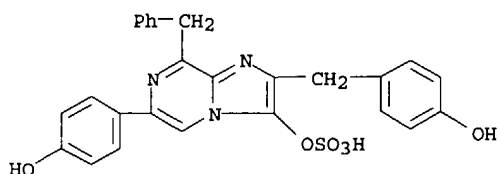


- RN 64750-83-0 HCAPLUS
- CN Imidazo[1,2-a]pyrazin-3-ol, 6-(4-hydroxyphenyl)-2,8-bis(phenylmethyl)-, 3-(hydrogen sulfate) (9CI) (CA INDEX NAME)

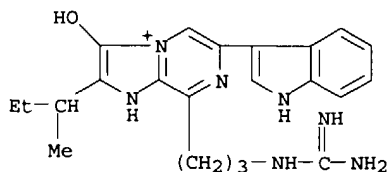


- L28 ANSWER 14 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN
- AN 1975:405600 HCAPLUS
- DN 83:5600
- ED Entered STN: 12 May 1984
- TI Chemical nature of bioluminescence systems in coelenterates

AU Shimomura, Osamu; Johnson, Frank H.  
 CS Dep. Biol., Princeton Univ., Princeton, NJ, USA  
 SO Proceedings of the National Academy of Sciences of the United States of America (1975), 72(4), 1546-9  
 CODEN: PNASA6; ISSN: 0027-8424  
 DT Journal  
 LA English  
 CC 12-13 (Nonmammalian Biochemistry)  
 AB Anal. of substances involved in light-emitting reactions among bioluminescent coelenterates revealed a pronounced uniformity in the structural features of initial reactants, i.e., luciferins and photoprotein chromophores, as well as the light-emitter product. This product is structurally identical among the different classes of coelenterates; i.e., Hydrozoa (the jellyfish, Aequorea), Anthozoa (the sea cactus, Cavernularia; sea pansy, Renilla; and sea pen, Leioptilus), and very likely also the Scyphozoa (the jellyfish, Pelagia). In each of these instances the reaction product, 2-(p-hydroxyphenylacetyl)amino-3-benzyl-5-(p-hydroxyphenyl) pyrazine, is the actual light-emitter, whether it occurs in a Ca<sup>2+</sup>-triggered photoprotein type of luminescence or in a luciferin-luciferase type. The evidence indicates that in certain coelenterates, e.g., Cavernularia, these 2 types are equally significant, whereas in others (Renilla and Leioptilus) the luciferin-luciferase type predominates over the Ca-triggerable photoprotein type. Only the photoprotein type functions in the luciferaseless jellyfish, Aequorea. In all instances investigated, the structure of the light-emitter prior to the luminescence reaction appears to be essentially the same as that of the chromophore of unreacted aequorin. The product of the luminescence reaction is absent in exts. of nonluminous species. However, a product very similar to that of luminescent coelenterates occurs also in representatives of other phyla, including the cephalopod molluscs, e.g., the "firefly squid" Watasenia and probably various ctenophores as well.  
 ST bioluminescence coelenterate hydroxyphenylacetylaminobenzylhydroxyphenyl pyrazine; pyrazine deriv bioluminescence coelenterate  
 IT Luminescence  
     (bio-, of coelenterates, (hydroxyphenylacetyl)aminobenzyl(hydroxyphenyl) pyrazine in)  
 IT Aequorea aequorea  
     Cavernularia obesa  
     Coelenterate  
     Leioptilus  
     Leptogorgia virgulata  
     Renilla  
     (bioluminescence of, (hydroxyphenylacetyl)aminobenzyl(hydroxyphenyl) pyrazine in)  
 IT Nomenclature, new natural products  
     (coelenteramide)  
 IT Nomenclature, new natural products  
     (coelenterazine)  
 IT Luciferins  
     RL: BIOL (Biological study)  
     (sulfate, of bioluminescence species, product of)  
 IT 50611-86-4 55779-48-1  
     RL: BIOL (Biological study)  
     (in bioluminescence, in coelenterates)  
 IT 37156-84-6 55779-47-0  
     RL: BIOL (Biological study)  
     (in calcium-induced luminescence of coelenterates)  
 IT 55779-47-0  
     RL: BIOL (Biological study)  
     (in calcium-induced luminescence of coelenterates)  
 RN 55779-47-0 HCAPLUS  
 CN Imidazo[1,2-a]pyrazin-3-ol, 6-(4-hydroxyphenyl)-2-[(4-hydroxyphenyl)methyl]-8-(phenylmethyl)-, 3-(hydrogen sulfate) (9CI) (CA INDEX NAME)



L28 ANSWER 15 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1973:145460 HCAPLUS  
 DN 78:145460  
 ED Entered STN: 12 May 1984  
 TI Exchange of oxygen between solvent water and the carbon dioxide produced in Cypridina bioluminescence  
 AU Shimomura, Osamu; Johnson, Frank H.  
 CS Biol. Dep., Princeton Univ., Princeton, NJ, USA  
 SO Biochemical and Biophysical Research Communications (1973), 51(3), 558-63  
 CODEN: BBRCA9; ISSN: 0006-291X  
 DT Journal  
 LA English  
 CC 12-2 (Nonmammalian Biochemistry)  
 AB Bioluminescent oxidation of Cypridina luciferin yields CO<sub>2</sub> besides oxyluciferin and light. The exchange of O between the CO<sub>2</sub> and H<sub>2</sub>O of the solvent becomes significant when <1.μmole of luciferin is reacted in 4 ml of buffer solution, and the exchange O in CO<sub>2</sub> markedly increases by decreasing the amount of luciferin. Such an exchange is to be expected in any such system which produces CO<sub>2</sub> in aqueous solution, and must be taken in to account in interpreting the results of expts.  
 ST luciferin oxidn bioluminescence; Cypridina bioluminescence  
 IT Luminescence  
 (bio-, luciferin oxidation in)  
 IT Cypridina  
 (luminescence of, oxygen exchange between carbon dioxide and water in)  
 IT Exchange reaction  
 (of oxygen, between carbon dioxide and water in Cypridina bioluminescence)  
 IT 7782-44-7, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (exchange reaction of, between carbon dioxide and water in Cypridina bioluminescence)  
 IT 7732-18-5  
 RL: BIOL (Biological study)  
 (exchange reactions of oxygen in, with carbon dioxide, in Cypridina bioluminescence)  
 IT 124-38-9, reactions  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (exchange reactions of oxygen in, with water, in Cypridina bioluminescence)  
 IT 26008-71-9  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (oxidation of, in bioluminescence)  
 IT 26008-71-9  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (oxidation of, in bioluminescence)  
 RN 26008-71-9 HCAPLUS  
 CN 1H-Imidazo[1,2-a]pyrazin-4-ium, 8-[3-[(aminoiminomethyl)amino]propyl]-3-hydroxy-6-(1H-indol-3-yl)-2-(1-methylpropyl)-, bromide, monohydrobromide (9CI) (CA INDEX NAME)



● Br<sup>-</sup>

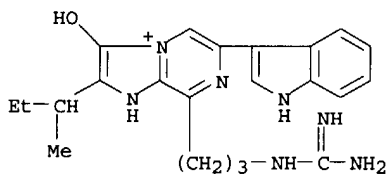
● HBr

L28 ANSWER 16 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1970:432730 HCAPLUS

Searched by Noble Jarrell



DN 73:32730  
 ED Entered STN: 12 May 1984  
 TI Chemistry of bioluminescence  
 AU Goto, Toshio  
 CS Dep. Agr. Chem., Nagoya Univ., Nagoya, Japan  
 SO Pure and Applied Chemistry (1968), 17(3-4), 421-41  
 CODEN: PACHAS; ISSN: 0033-4545  
 DT Journal; General Review  
 LA English  
 CC 9 (Nonmammalian Biochemistry)  
 AB The bioluminescence kinetics and mechanisms of *Cypridina hilgendorffii* luciferin and related compds. is reviewed. 40 refs.  
 ST *Cypridina* bioluminescence review; bioluminescence kinetics; kinetics bioluminescence; luciferin luciferase kinetics; review bioluminescence luciferin  
 IT Luminescence  
 IT (bio-, of *Cypridina hilgendorffii*)  
 IT *Cypridina*  
 IT (hilgendorffii, bioluminescence of)  
 IT 26008-71-9  
 RL: PRP (Properties)  
 IT (bioluminescence of, of *Cypridina hilgendorffii*)  
 IT 26008-71-9  
 RL: PRP (Properties)  
 IT (bioluminescence of, of *Cypridina hilgendorffii*)  
 RN 26008-71-9 HCAPLUS  
 CN 1H-Imidazo[1,2-a]pyrazin-4-ium, 8-[3-[(aminoiminomethyl)amino]propyl]-3-hydroxy-6-(1H-indol-3-yl)-2-(1-methylpropyl)-, bromide, monohydrobromide (9CI) (CA INDEX NAME)

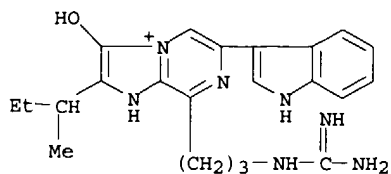


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L28 ANSWER 17 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1970:107330 HCAPLUS  
 DN 72:107330  
 ED Entered STN: 12 May 1984  
 TI Enzyme catalyzed oxidation of *Cypridina* luciferin  
 AU Stone, Henry  
 CS Princeton Univ., Princeton, NJ, USA  
 SO (1969) 80 pp. Avail.: 69-14,438  
 From: Diss. Abstr. Int. B 1969, 30(3), 1020-1  
 DT Dissertation  
 LA English  
 CC 3 (Enzymes)  
 AB Unavailable  
 ST *Cypridina* luciferin oxidn; luciferin enzymic oxidn  
 IT Enzymes  
 RL: BIOL (Biological study)  
 IT (luciferin-oxidizing, of *Cypridina*)  
 IT 26008-71-9  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 IT (oxidation of, enzymic)  
 IT 26008-71-9  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 IT (oxidation of, enzymic)  
 RN 26008-71-9 HCAPLUS  
 CN 1H-Imidazo[1,2-a]pyrazin-4-ium, 8-[3-[(aminoiminomethyl)amino]propyl]-3-

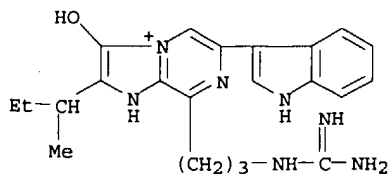
hydroxy-6-(1H-indol-3-yl)-2-(1-methylpropyl)-, bromide, monohydrobromide  
(9CI) (CA INDEX NAME)



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● HBr

L28 ANSWER 18 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN  
AN 1970:62631 HCAPLUS  
DN 72:62631  
ED Entered STN: 12 May 1984  
TI Bioluminescence and mechanism of luminescence  
AU Got, Toshio  
CS Nagoya Univ., Nagoya, Japan  
SO Kagaku to Seibutsu (1969), 7(8), 445-51  
CODEN: KASEAA; ISSN: 0453-073X  
DT Journal; General Review  
LA Japanese  
CC 2 (General Biochemistry)  
AB A review. Mechanism of chemiluminescence was outlined with special reference to the formation of an intermediate hydroperoxide anion and its decomposition through 4-membered ring peroxide into carbonyl compound in singlet excited state, and illustrated by Cypridina luciferin. 28 refs.  
ST bioluminescence review; review bioluminescence; luminescence review  
IT Luminescence  
(bio-, mechanism of)  
IT 26008-71-9  
RL: PRP (Properties)  
(luminescence of, mechanism of)  
IT 26008-71-9  
RL: PRP (Properties)  
(luminescence of, mechanism of)  
RN 26008-71-9 HCAPLUS  
CN 1H-Imidazo[1,2-a]pyrazin-4-ium, 8-[3-[(aminoiminomethyl)amino]propyl]-3-hydroxy-6-(1H-indol-3-yl)-2-(1-methylpropyl)-, bromide, monohydrobromide  
(9CI) (CA INDEX NAME)



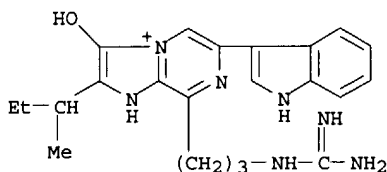
● Br<sup>-</sup>

● HBr

L28 ANSWER 19 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN

Searched by Noble Jarrell

AN 1968:46251 HCAPLUS  
 DN 68:46251  
 ED Entered STN: 12 May 1984  
 TI Bioluminescence. Cypridina luciferin  
 AU Hirata, Yoshimasa; Goto, Toshio  
 CS Nagoya Univ., Nagoya, Japan  
 SO Kagaku (Tokyo, Japan) (1967), 37(12), 640-6  
 CODEN: KAGTAT; ISSN: 0022-7625  
 DT Journal  
 LA Japanese  
 CC 2 (General Biochemistry)  
 GI For diagram(s), see printed CA Issue.  
 AB The scheme of bioluminescence reaction of luciferin can be represented:  
 luciferin + O<sub>2</sub> -(luciferase).fwdarw. oxyluciferin +hv. Oxyluciferin was  
 gradually decomposed to etioluciferin (I). From further studies on the  
 structure of luciferin, the new structure II was proposed. Attempts to  
 synthesize II gave a very poor yield.  
 ST BIOLUMINESCENCE LUCIFERIN; ETIOLUCIFERIN; LUCIFERIN STRUCTURE ACTION;  
 LUMINESCENCE LUCIFERIN  
 IT Luminescence  
 (bio-, of luciferin, intermediates in)  
 IT Cypridina  
 (luciferin of, bioluminescence of, intermediates in)  
 IT Molecular structure  
 (of luciferin)  
 IT 19321-05-2  
 RL: BIOL (Biological study)  
 (luciferin (cypridina) identity with)  
 IT 19321-05-2  
 RL: BIOL (Biological study)  
 (luciferin (cypridina) identity with)  
 RN 19321-05-2 HCAPLUS  
 CN 1H-Imidazo[1,2-a]pyrazin-4-ium, 2-sec-butyl-8-(3-guanidinopropyl)-3-  
 hydroxy-6-indol-3-yl-, bromide, monohydrobromide (8CI) (CA INDEX NAME)



● Br<sup>-</sup>

● HBr

L28 ANSWER 20 OF 20 HCAPLUS COPYRIGHT 2004 ACS on STN  
 AN 1967:432674 HCAPLUS  
 DN 67:32674  
 ED Entered STN: 12 May 1984  
 TI Structure of Cypridina luciferin  
 AU Kishi, Yoshito; Goto, Toshio; Hirata, Yoshimasa; Shimomura, Osamu;  
 Johnson, Frank Harris  
 CS Fac. Sci., Nagoya Univ., Nagoya, Japan  
 SO Biolumin. Prog., Proc. Conf. (1966), Meeting Date 1965, 89-113  
 CODEN: 16HSAG  
 DT Conference  
 LA English  
 CC 28 (Heterocyclic Compounds (More Than One Hetero Atom))  
 GI For diagram(s), see printed CA Issue.  
 AB Luciferin yields oxyluciferin (I) and etioluciferin (II) when treated with  
 luciferase-O or NH<sub>3</sub>-O. The former can be converted to the latter by acid  
 treatment. Treatment of II with Ba(OH)<sub>2</sub> gives etioluciferamine. N.M.R.  
 spectra and high-resolution mass spectra as well as chemical data confirm the  
 structures of these compds. On the basis of structure II, the structure I  
 can be assigned to oxyluciferin. The structure III is assigned to

luciferin hydrobromide and IV to luciferin hydrochloride. These structures comprise tryptamine, arginine, and isoleucine moieties.

ST STRUCTURE CYPRIDINA LUCIFERIN; LUCIFERIN CYPRIDINA STRUCTURE; ARGININE; ISOLEUCINE; ETIOLUCIFERIN; CYPRIDINA LUCIFERIN STRUCTURE

IT Cypridina  
(luciferin of, structure of)

IT 1H-Imidazo[1,2-a]pyrazin-4-ium, 2-sec-butyl-8-(3-guanidinopropyl)-3-hydroxy-6-indol-3-yl-, hydroxide  
Guanidine, [3-(2-sec-butyl-3,7-dihydro-6-indol-3-yl-3-oxoimidazo[1,2-a]pyrazin-8-yl)propyl]-  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(as structure of luciferin)

IT Luciferin  
Luciferin, bromide, hydrobromide  
Luciferin, hydroxide  
RL: PRP (Properties)  
(structure of)

IT 7256-95-3  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(as structure of etioluciferamine)

IT 7269-75-2  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(as structure of etioluciferin)

IT 19321-05-2  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(as structure of luciferin hydrobromide)

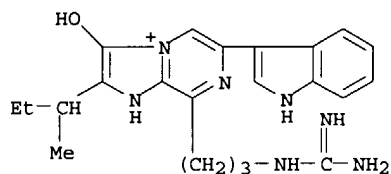
IT 10104-19-5  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(as structure of oxyluciferin)

IT 7256-95-3 7269-75-2 17297-78-8  
RL: PRP (Properties)  
(structure of)

IT 19321-05-2  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(as structure of luciferin hydrobromide)

RN 19321-05-2 HCAPLUS

CN 1H-Imidazo[1,2-a]pyrazin-4-ium, 2-sec-butyl-8-(3-guanidinopropyl)-3-hydroxy-6-indol-3-yl-, bromide, monohydrobromide (8CI) (CA INDEX NAME)



● Br<sup>-</sup>

● HBr

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